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IBM Technical Disclosure Bulletins

Term:

(ep-1364995-\$.did. or de-10225048-\$.did. or
gb-2377706-\$.did. or jp-2001106645-\$.did. or
jp-2001106644-\$.did.)

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20

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jp-2001106645-\$.did. or jp-2001106644-\$.did.)

7 L1

END OF SEARCH HISTORY

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L1: Entry 2 of 7

File: JPAB

Apr 17, 2001

PUB-NO: JP02001106644A
DOCUMENT-IDENTIFIER: JP 2001106644 A
TITLE: HYDROPHENANTHRENE DERIVATIVE

PUBN-DATE: April 17, 2001

INVENTOR-INFORMATION:

NAME

COUNTRY

OGAWA, SHINJI
TAKEHARA, SADA
ONISHI, HIROYUKI
TAKEUCHI, KIYOBUMI
TAKATSU, HARUYOSHI
GERHARD, GURAAE
FRINGS, RAINER BRUNO
PITHART, CORNELIA

INT-CL (IPC): C07 C 25/22; C07 C 25/13; C07 C 43/225; C07 C 255/50; C09 K 19/32; C09 K 19/34; G02 F 1/13

ABSTRACT:

PROBLEM TO BE SOLVED: To obtain a compound capable of effectively improving the stability of the liquid crystal phase within the temperature range, especially low temperatures by adding thereof, a liquid crystal composition and a liquid crystal display element having a wide temperature range by using the compound.

SOLUTION: This hydrophenanthrene derivative is represented by formula (I). The nematic liquid crystal composition and liquid crystal display element comprise the derivative. One example of the derivative is represented by formula (II) (R is C3H7).

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L1: Entry 1 of 7

File: JPAB

Apr 17, 2001

PUB-NO: JP02001106645A

DOCUMENT-IDENTIFIER: JP 2001106645 A

TITLE: CONDENSED RING COMPOUND

PUBN-DATE: April 17, 2001

INVENTOR-INFORMATION:

NAME

COUNTRY

OGAWA, SHINJI

TAKEHARA, SADA0

ONISHI, HIROYUKI

TAKATSU, HARUYOSHI

INT-CL (IPC): C07 C 25/22; C07 C 43/225; C07 C 255/52; C07 C 255/55; C09 K 19/32;
C09 K 19/34; G02 F 1/13

ABSTRACT:

PROBLEM TO BE SOLVED: To obtain a compound which is a phenanthrene derivative and a fluorene derivative capable of extending the temperature range of the liquid crystal phase and reducing the threshold voltage of a display element by adding thereof, a liquid crystal composition and the liquid crystal display element by using the compound.

SOLUTION: This new compound is represented by general formula (I) [rings A and C denote each trans-1,4-cyclohexylene group, 1,4-phenylene group, 1,4-cyclohexenylene group, 1,4-bicyclo(2.2.2)octylene group, piperidine-1,4-diyl group, naphthalene-2,6-diyl group, trans-dehydronaphthalene-trans-2,6-diyl group or 1,2,3,4-tetrahydronaphthalene-2,6-diyl group or the like; and ring B denotes phenanthrene-2,7-diyl group, 9,10-dihydrophenanthrene-2,7-diyl group or fluorene-2,7-diyl group or the like] or the like. The nematic liquid crystal composition comprises the compound.

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L1: Entry 7 of 7

File: DWPI

Sep 25, 2002

DERWENT-ACC-NO: 2001-226501

DERWENT-WEEK: 200305

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TITLE: Fused ring compound used in liquid crystal compositions for active matrix driven liquid crystal display elements and super-twisted nematic liquid crystal elements

INVENTOR: FRINGS, R B; FUGGER, C ; GRAHE, G ; KAWARA, T ; OGAWA, S ; OHNISHI, H ; PITHART, C ; TAKATSU, H ; TAKEHARA, S ; TAKEUCHI, K

PRIORITY-DATA: 1999JP-0219855 (August 3, 1999)

PATENT-FAMILY:

PUB-NO	PUB-DATE	LANGUAGE	PAGES	MAIN-IPC
CN 1371347 A	September 25, 2002		000	C07C013/60
WO 200110803 A1	February 15, 2001	J	270	C07C013/60
<u>JP 2001106644 A</u>	April 17, 2001		080	C07C025/22
AU 9956488 A	March 5, 2001		000	C07C013/60
EP 1201632 A1	May 2, 2002	E	000	C07C013/60
KR 2002014842 A	February 25, 2002		000	C07C013/60

INT-CL (IPC): C07 C 13/60; C07 C 25/13; C07 C 25/22; C07 C 25/24; C07 C 39/17; C07 C 43/225; C07 C 49/675; C07 C 255/50; C07 C 255/55; C09 K 19/32; C09 K 19/34; G02 F 1/13

ABSTRACTED-PUB-NO: WO 200110803A

BASIC-ABSTRACT:

NOVELTY - Fused ring compound is used in liquid crystal compositions for active matrix driven liquid crystal display elements and super-twisted nematic liquid crystal elements.

DETAILED DESCRIPTION - Fused ring compound is of formula (I)

R = 1-16C alkyl or alkoxy group, 2-16C alkenyl group, 3-16C alkenyloxy group, or 1-12C alkyl group substituted by 1-10C alkoxy group, all of which being optionally substituted by halogen and being optionally racemic with optical activity generated by the asymmetric carbon in the substituent or branching;

ring A and ring C = trans-1,4-cyclohexylene group in which 1 CH₂ group or at least 2 adjoining -CH₂ groups present in the group is exchanged with -O- and/or -S-, 1,4-phenylene group in which 1 CH group or at least 2 adjoining -CH groups present in the group is exchanged with -N=, 1,4-cyclohexylene group, 1,4-bicyclo(2,2,2)octylene group, piperidine-1,4-diyl group, naphthalene-2,6-diyl group, trans-decahydronaphthalene-trans-2,6-diyl group or 1,2,3,4-tetrahydronaphthalene-2,6-diyl group, all being optionally substituted with amino groups or halogen;

ring B = a group of formula (1)-(9);

X1, X3, X4, X5, X6, X8, X9, and X10 = H, Cl or F, where

(a) in (1) and (2), at least 1 of X1, X8, X9 and X10 = Cl or F when at least 1 of X3-6 = F and the rest = H;

(b) in (1) and (2), at least 1 of X3-6 = Cl or F when at least 1 of X1, X8, X9 or X10 = F and the rest = H;

(c) = H atoms on the rings (3)-(9) are optionally substituted by amino groups or halogen;

L1-2 = -CH₂-CH₂-, -C equivalent to C-, -(CH₂)₄-, -CF=CF-, -OCH₂-, -CH₂O-, -OCF₂-, -CF₂O-, -CO₂-, -OCO-, -CH=N-N=CH-, -CH=CH-CH₂-CH₂-, -CH₂-CH₂-CH=CH- or a single bond;

m and n = 0, 1 or 2;

m + n at most 2; when m or n = 2, at least 1 of L1-2 = a single bond; Y = H, F, Cl, trifluoromethoxy group, difluoromethane, trifluoromethyl, 3,3,3-trifluoroethoxy, cyano, 1-16C linear alkyl, 2-16C linear alkenyl, 1-12C linear alkenyloxy or 2-16C linear alkenyloxy.

The following are excluded; (i) ring B = (2), m and n = 0, R = alkyl, and Y = alkyl; (ii) ring B = (3), m and n = 0, R = alkyl and Y = alkoxy; (iii) ring B = (4), m and n = 0, R = alkyl and Y = alkyl or cyano; (iv) ring B = (8), m and n = 0, R = alkyl and Y = alkyl; (v) ring B = (4) m = 0, n = 1, ring C = 1,4-phenylene, L2 = CO₂-, R = alkyl, and Y = alkyl, alkoxy or cyano; (vi) ring B = (4), m = 0, n = 1, ring C = 1,4-cyclohexylene, L2 = -CO₂-, R = alkyl and Y = alkyl; (vii) ring B = (2), m = 0, n = 1, ring C = 1,4-cyclohexylene, L2 = -CO₂-, R = alkyl, and Y = alkyl; (viii) ring B = (1), X₉ and X₁₀ = F; (ix) ring B = (3), X₃₋₆ = F. INDEPENDENT CLAIMS are also included for (alpha) a liquid crystal composition containing at least 1 compound (I); (beta) a liquid crystal element using the composition.

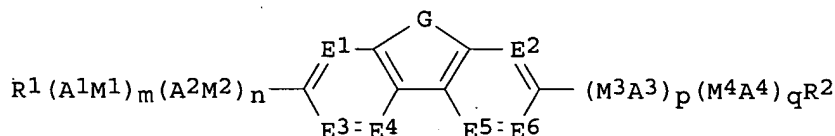
USE - (I) are used in liquid crystal composition for active matrix driven liquid crystal display elements and super-twisted nematic liquid crystal display elements.

ADVANTAGE - (I) is easily produced and has excellent compatibility with a mother liquid currently used as a nematic liquid crystal, and shows reduced precipitation at a low temperature. The addition of a small amount of (I) to the mother liquid crystal expands the temperature range for liquid crystallinity without harming various properties as a liquid crystal material. (I) has a wide range of working temperature.

AN 1998:424211 CAPLUS
 DN 129:89046
 TI Derivatives of 9,9-difluoro-9,10-dihydrophenanthrene for **liquid crystal** mixtures
 IN Schmidt, Wolfgang; Manero, Javier
 PA Hoechst Research & Technology Deutschland G.m.b.H. & Co. K.-G., Germany; Schmidt, Wolfgang; Manero, Javier
 SO PCT Int. Appl., 44 pp.
 CODEN: PIXXD2
 DT Patent
 LA German
 IC ICM C07C043-225
 ICS C09K019-32; C09K019-34; C09K019-40; C07F007-08; C07C069-75; C07C069-96; C07D213-64
 CC 76-8 (Electric Phenomena)
 Section cross-reference(s): 25, 28, 74, 75

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9827043	A1	19980625	WO 1997-EP7057	19971216
	W: JP, KR, US				
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	DE 19653010	A1	19980625	DE 1996-19653010	19961219
	EP 946477	A1	19991006	EP 1997-953829	19971216
	EP 946477	B1	20020731		
	R: DE				
PRAI	DE 1996-19653010	A	19961219		
	WO 1997-EP7057	W	19971216		
OS	MARPAT 129:89046				
GI					



AB I are suitable as components for **liq. crystal** mixts., in particular ferroelec. mixts., which are suitable for electrooptical display devices. In I G = -CF2CH2-; E1, E2, E3, E4, E5, E6 are identical or different and = -CH-, -CF- or -N-; and R1(A1M1)m(A2M2)n, (M3A3)p(M4A4)qR2 are mesogenic radicals. R1 and R2 are identical or different and = H, F, Cl, CF3, OCF3, or CN, or = C1-20 alkyl group with different substituents; M1-4 are identical or different and = CO2, OCO, COS, SCO, CSO, OCS, CH2O, OCH2, CH2S, SCH2, C2H2, C2, (CH2)2CO2, or OCO(CH2)2. A1-4 are identical or different 1,4-phenylenes, pyrazine-2,5-diyls, pyridazine-2,6-diyls, pyridine-2,5-diyls, pyrimidine-2,5-diyls, 1,4-cyclohexylenes, (1,3,4)-thiadiazole-2,5-diyls, 1,3-dioxane-2,5-diyls, 1,3-dithiane-2,5-diyls, 1,3-thiazole-2,4-diyls, 1,3-thiazole-2,5-diyls, thiophene-2,4-diyls, thiophene-2,5-diyls, piperazine-1,4-diyls, piperazine-2,5-diyls, or 1-(C1-C4)alkyl-1-silacyclohexylene-1,4-diyls with different or no substituents such as F, Cl, CN and in some cases Me. M, n, p, and q are 0 or 1. I does not contain more than 4 5-member or higher ring systems. The prepn. of these compds. is described.

ST fluorodihydrophenanthrene deriv ferroelec mesophase display
 IT **Liquid crystal** displays
 Liquid mixtures
 (difluorodihydrophenanthrene derivs. for ferroelec. **liq. crystal** mixts. for electrooptical displays)
 IT **Liquid crystals**

WEST

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L1: Entry 4 of 7

File: EPAB

Dec 12, 2002

PUB-NO: DE010225048A1

DOCUMENT-IDENTIFIER: DE 10225048 A1

TITLE: New stable, liquid crystalline fluorinated phenanthrene or 9,10-dihydrophenanthrene derivatives having a high clear point, useful in liquid crystalline media for electrooptical displays

PUBN-DATE: December 12, 2002

INVENTOR-INFORMATION:

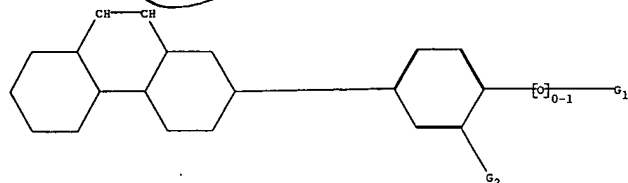
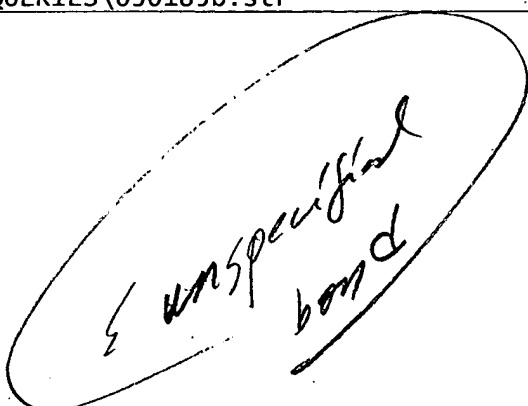
NAME	COUNTRY
BREMER, MATTHIAS	DE
PAULUTH, DETLEF	DE
HECKMEIER, MICHAEL	DE
DUEBAL, HANS-ROLF	DE
HORNUNG, BARBARA	DE
SCHMIDT, WOLFGANG	DE
WINGEN, RAINER	DE

INT-CL (IPC): C07 C 25/18; C07 C 25/24; C07 C 13/62; C07 C 43/225; C07 C 69/00; C07 C 255/00; C07 C 331/02; C07 C 331/16; C07 C 381/00; C09 K 19/06; G02 F 1/137; G09 F 9/35

EUR-CL (EPC): C09K019/42; C07C013/573, C07C017/361, C07C017/361, C07C025/22, C07C025/24, C07C045/00, C07C255/50, C07C255/54, C09K019/32

ABSTRACT:

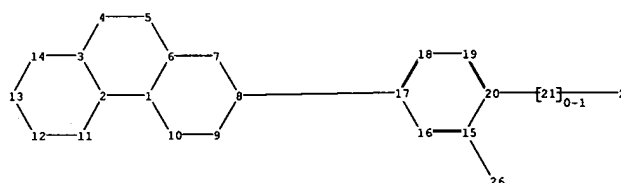
CHG DATE=20030507 STATUS=N>Optionally fluorinated phenanthrene or 9,10-dihydrophenanthrene derivatives (I), carrying an alkyl or alkylene chain (optionally bonded via linking groups) in the 2-position, are new. Liquid crystalline phenanthrene or dihydrophenanthrene derivatives of formula (I) are new. R = 1-15C alkyl or 2-15C alkenyl (both optionally substituted by one CN or CF₃ or by one or more halo; and optionally having one or more CH₂ groups replaced by O, S, CC, COO or OCO, provided that O atoms are not directly bonded to each other); A1 = 1,4-cyclohexenylene or 1,4-cyclohexylene (both optionally having 1 or 2 non-adjacent CH₂ groups replaced by O or S) or 1,4-phenylene (optionally having 1 or 2 CH groups replaced by N), all optionally substituted by one or more F; Z1 = COO, OCO, CF₂O, OCF₂, CH₂O, OCH₂, CH₂CH₂, C₂F₄, CH=CH, CC or a direct bond; Y = H, F, Cl, CN, SF₅, NCS or SCN; or 1-5C alkyl, 2-5C alkenyl, 2-5C alkenyloxy or 1-5C alkoxy, all mono- or polysubstituted by halo; G = CH₂CH₂, CH=CF or CH=CH; L1 - L5 = H or F; m = 0-2. An Independent claim is included for a liquid crystalline medium (A) containing at least two mesogenic compounds, which contains at least one compound (I).



$$N = 0$$

$$M = 1$$

$$L^2 = \text{single bond}$$



chain nodes :

21 22 26

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

chain bonds :

8-17 15-26 20-21 21-22

ring bonds :

1-2 1-6 1-10 2-3 2-11 3-4 3-14 4-5 5-6 6-7 7-8 8-9 9-10 11-12 12-13 13-14
15-16 15-20 16-17 17-18 18-19 19-20

exact/norm bonds :

15-26 20-21 21-22

exact bonds :

1-2 1-6 1-10 2-3 2-11 3-4 3-14 4-5 5-6 6-7 7-8 8-9 8-17 9-10 11-12 12-13
13-14

normalized bonds :

15-16 15-20 16-17 17-18 18-19 19-20

isolated ring systems :

containing 1 :

G1:Cl,F,CF2,CF3,C,H,O,CH3,Et,n-Pr,CN

G2:H,F

Match level :

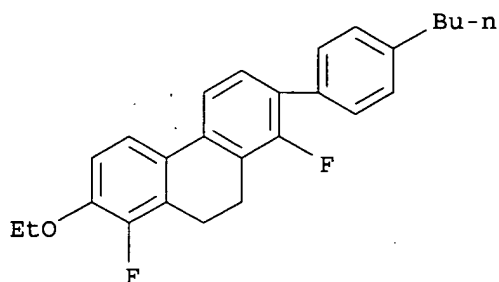
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS
22:CLASS 26:CLASS

=> dis 2, 10, 106, 148 all

L6 ANSWER 2 OF 500 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 603991-30-6 REGISTRY
 CN Phenanthrene, 2-(4-butylphenyl)-7-ethoxy-1,8-difluoro-9,10-dihydro- (9CI)
 (CA INDEX NAME)
 FS 3D CONCORD
 MF C26 H26 F2 O
 SR CA
 LC STN Files: CA, CAPLUS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1
C6-C6-C6	C6-C6-C6	6-6-6	C14	2404.11.86	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1000000.0	pH 1	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 4	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 7	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 8	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 10	(1) ACD
Boiling Point (BP)	525.4+/-35.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVP)	76.94+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	281.7+/-39.3 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	6		(1) ACD
H acceptors (HAC)	1		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	5233135	pH 1	(1) ACD
Koc (KOC)	5233135	pH 4	(1) ACD
Koc (KOC)	5233135	pH 7	(1) ACD
Koc (KOC)	5233135	pH 8	(1) ACD
Koc (KOC)	5233135	pH 10	(1) ACD
logD (LOGD)	9.82	pH 1	(1) ACD
logD (LOGD)	9.82	pH 4	(1) ACD
logD (LOGD)	9.82	pH 7	(1) ACD
logD (LOGD)	9.82	pH 8	(1) ACD
logD (LOGD)	9.82	pH 10	(1) ACD
logP (LOGP)	9.819+/-0.503		(1) ACD

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	392.48		(1) ACD
Vapor Pressure (VP)	1.33E-10 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD).

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 139:268384 CA
 TI Preparation of quaterphenyls and related compounds via combinatorial chemistry for use as liquid crystals
 IN Pauluth, Detlef; Kirsch, Peer; Baeuerle, Peter; Deeg, Oliver
 PA Merck Patent G.m.b.H., Germany
 SO Eur. Pat. Appl., 48 pp.
 CODEN: EPXXDW
 DT Patent
 LA German
 IC ICM C07F005-04
 ICS C07C025-18; C09K019-12
 CC 75-8 (Crystallography and Liquid Crystals)
 Section cross-reference(s): 25

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1346995	A1	20030924	EP 2003-3811	20030220
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	DE 10211597	A1	20031002	DE 2002-10211597	20020315
	JP 2003286208	A2	20031010	JP 2003-69260	20030314
PRAI	DE 2002-10211597		20020315		

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I and related compds. [X = single bond, CH₂CH₂, CH=CH, etc.; L = R, halo, OH, etc.; R = alkyl, alkenyl, acylalkyl, etc.; R₁, R₂ = H, F, Cl, etc.] were prep'd. For example, Suzuki coupling of terphenyl II, e.g., prep'd. from 1,2-difluorobenzene in 5-steps, and boronic acid III afforded quaterphenyl IV in 68% yield. Of note is the use of Suzuki coupling in combinatorial chem.

ST quaterphenyl prepn combinatorial chem suzuki coupling liq crystal

IT Combinatorial chemistry
 Liquid crystals
 Silylation
 Suzuki coupling reaction
 (prepn. of quaterphenyls and related compds. via combinatorial chem. for use as liq. crystals)

IT 98-80-6P 54156-71-7P 138871-01-9P 537013-51-7P 574755-30-9P
 574755-40-1P 574755-41-2P 603990-25-6P 603990-27-8P 603990-28-9P
 603990-30-3P 603990-31-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; prepn. of quaterphenyls and related compds. via

combinatorial chem. for use as liq. crystals)

IT 129738-34-7 163185-42-0 477557-80-5 603991-38-4 603991-39-5
603991-41-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(mixt. contg.; prepn. of quaterphenyls and related compds. via
combinatorial chem. for use as liq. crystals)

IT 3375-31-3
RL: CAT (Catalyst use); USES (Uses)
(prepn. of quaterphenyls and related compds. via combinatorial chem.
for use as liq. crystals)

IT 67-63-0, Isopropanol, uses 75-05-8, Acetonitrile, uses 123-91-1,
Dioxane, uses
RL: NUU (Other use, unclassified); USES (Uses)
(prepn. of quaterphenyls and related compds. via combinatorial chem.
for use as liq. crystals)

IT 75-77-4, Trimethylsilyl chloride, reactions 121-43-7 126-30-7
367-11-3, 1,2-Difluorobenzene 461-96-1, 1-Bromo-3,5-difluorobenzene
534-00-9 624-73-7, 1,2-Diiodoethane 2591-86-8, N-Formylpiperidine
5419-55-6 7790-99-0, Iodine chloride (ICl) 105931-73-5 134150-01-9,
4-Propylphenylboronic acid 603990-33-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of quaterphenyls and related compds. via combinatorial chem.
for use as liq. crystals)

IT 603-35-0P, Triphenylphosphine, preparation
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. of quaterphenyls and related compds. via combinatorial chem.
for use as liq. crystals)

IT 109-72-8, Butyl lithium, reactions 13400-13-0, Cesium fluoride 17194-0
0-2, Barium hydroxide
RL: RGT (Reagent); RACT (Reactant or reagent)
(prepn. of quaterphenyls and related compds. via combinatorial chem.
for use as liq. crystals)

IT 603990-35-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of quaterphenyls and related compds. via combinatorial chem.
for use as liq. crystals)

IT 138220-05-0P 138220-07-2P 326795-86-2P 478267-19-5P 478268-76-7P
500001-06-9P 574755-52-5P 574755-53-6P 574755-54-7P 574755-55-8P
574755-56-9P 574755-59-2P 574755-60-5P 574755-61-6P 574755-62-7P
574755-63-8P 574755-64-9P 574755-65-0P 574755-66-1P 574755-67-2P
574755-68-3P 574755-69-4P 574755-70-7P 574755-71-8P 574755-72-9P
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RL: SPN (Synthetic preparation); PREP (Preparation)
(product; prepn. of quaterphenyls and related compds. via combinatorial chem. for use as liq. crystals)

RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD

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- (2) Anon; PATENT ABSTRACTS OF JAPAN 1996, V1996(07)
- (3) Benneteau, B; TETRAHEDRON 1993, 47
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- (6) Coe, P; J FLUORINE CHEM 1998, 1, CAPLUS
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- (14) Hoechst Ag; DE 4426671 A 1996 CAPLUS
- (15) Ici Plc; EP 0470795 A 1992 CAPLUS
- (16) Kaufmann, D; CHEMISCHE BERICHTE 1987, 6, CAPLUS
- (17) Kiryanov, A; JOURNAL OF MATERIALS CHEMISTRY 2001, V11(12), P3068 CAPLUS
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- (19) Merck Patent Gmbh; WO 9001526 A 1990 CAPLUS
- (20) Merck Patent Gmbh; DE 4220082 A 1993 CAPLUS
- (21) Merck Patent Gmbh; DE 19933175 A 2000 CAPLUS
- (22) Merck Patent Gmbh; GB 2367058 A 2002 CAPLUS
- (23) Seiko Epson Corp; JP 08081416 A 1996 CAPLUS

L6 ANSWER 10 OF 500 REGISTRY COPYRIGHT 2003 ACS on STN

RN 478270-11-0 REGISTRY

CN Phenanthrene, 1,5-difluoro-2-(1,1,2,3,3,3-hexafluoropropoxy)-7-[4-(3E)-3-pentenylphenyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C28 H20 F8 O

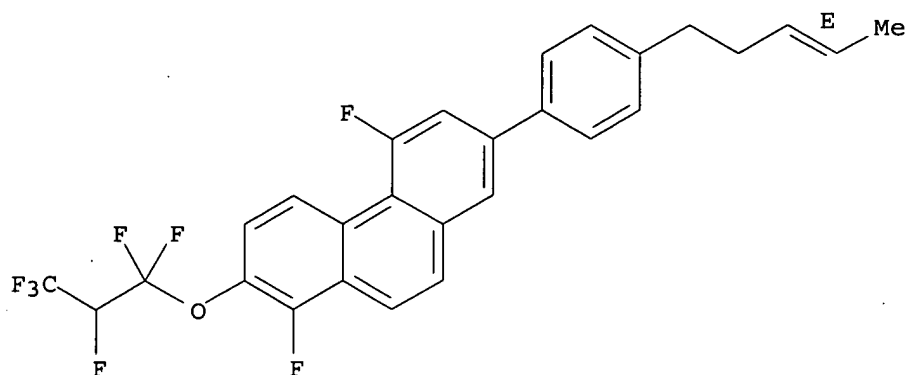
SR CA

LC STN Files: CA, CAPLUS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence Count
EA	ES	SZ	RF	RID	
C6	C6	6	C6	46.150.18	1
C6-C6-C6	C6-C6-C6	6-6-6	C14	2404.11.109	1

Double bond geometry as shown.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1000000.0	pH 1	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 4	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 7	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 8	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 10	(1) ACD
Boiling Point (BP)	529.2+/-35.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVP)	77.39+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	284.1+/-39.3 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	7		(1) ACD
H acceptors (HAC)	1		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	10000000.0	pH 1	(1) ACD
Koc (KOC)	10000000.0	pH 4	(1) ACD
Koc (KOC)	10000000.0	pH 7	(1) ACD
Koc (KOC)	10000000.0	pH 8	(1) ACD
Koc (KOC)	10000000.0	pH 10	(1) ACD
logD (LOGD)	10.51	pH 1	(1) ACD
logD (LOGD)	10.51	pH 4	(1) ACD
logD (LOGD)	10.51	pH 7	(1) ACD
logD (LOGD)	10.51	pH 8	(1) ACD
logD (LOGD)	10.51	pH 10	(1) ACD
logP (LOGP)	10.507+/-0.866		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	524.45		(1) ACD
Vapor Pressure (VP)	9.41E-11 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

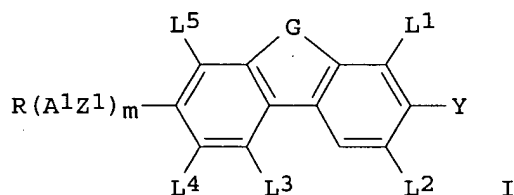
AN 138:31093 CA
TI Fluorinated (dihydro)phenanthrene derivatives and their use in liquid crystalline media

IN Bremer, Matthias; Pauluth, Detlef; Heckmeier, Michael; Duebal, Hans-Rolf;
Hornung, Barbara; Schmidt, Wolfgang; Wingen, Rainer
PA Merck Patent G.m.b.H., Germany
SO Ger. Offen., 124 pp.
CODEN: GWXXBX
DT Patent
LA German
IC ICM C07C025-18
ICS C07C025-24; C07C013-62; C07C043-225; C07C069-00; C07C255-00;
C07C331-02; C07C331-16; C07C381-00; C09K019-06; G02F001-137;
G09F009-35
CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other
Reprographic Processes)
Section cross-reference(s): 75

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 10225048	A1	20021212	DE 2002-10225048	20020606
	GB 2377706	A1	20030122	GB 2002-13110	20020607
	JP 2003096003	A2	20030403	JP 2002-166852	20020607
PRAI	DE 2001-10127482		20010607		
	DE 2001-10136965		20010728		

GI



AB The invention relates to a liq. cryst. (dihydro)phenanthrene derivate of the formula I (R = C1-15-alkyl, alkenyl; A1 = 1,4-cyclohexenylene, 1,4-cyclohexylene, 1,4-phenylene; Z1 = -COO-, -OCO-, -CF2O-, -OCF2-, -CH2O-, -OCH2-, -CH2CH2-, -C2F4-, -CH:CH-, -C.tplbond.C-, single bond; Y = H, F, Cl, CN, SF5, NCS, SCN, C1-5-alkyl, alkenyl, alkenyloxy, alkoxy; G = -CH2CH2-, -CH:CF-, -CH:CH-; L1-5 = H, F; m = 0, 1), as well as liq. cryst. media, contg. at least the above (dihydro)phenanthrene deriv., and electrooptical displays contg. the above liq. crystal media. The (dihydro)phenanthrene deriv. were synthesized.

ST fluorinated phenanthrene dihydrophenanthrene synthesis nematic liq crystal mixt display

IT 76802-59-0 76802-61-4 81711-13-9 84540-37-4 84816-56-8
92263-41-7 94840-77-4 97398-75-9 106349-49-9 116020-44-1
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RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(liq. crystal mixt. contg. fluorinated (dihydro)phenanthrene derivs. for liq. crystal display)

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RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

IT 4009-98-7, Methoxymethyltriphenylphosphoniumchloride 132123-39-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

IT 478264-03-8P 478264-04-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

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RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
 (prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

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	478268-51-8P	478268-52-9P	478268-53-0P	478268-54-1P	478268-55-2P
	478268-56-3P	478268-58-5P	478268-59-6P	478268-60-9P	478268-61-0P
	478268-62-1P	478268-63-2P	478268-64-3P	478268-65-4P	478268-66-5P
	478268-67-6P	478268-68-7P	478268-69-8P	478268-70-1P	478268-71-2P
	478268-72-3P	478268-73-4P	478268-74-5P	478268-75-6P	478268-77-8P
	478268-78-9P	478268-79-0P	478268-80-3P	478268-81-4P	478268-82-5P
	478268-83-6P	478268-84-7P	478268-85-8P	478268-86-9P	478268-87-0P
	478268-88-1P	478268-89-2P			

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
 (prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

IT	478268-90-5P	478268-91-6P	478268-93-8P	478268-94-9P	478268-95-0P
	478268-96-1P	478268-97-2P	478268-98-3P	478268-99-4P	478269-00-0P
	478269-01-1P	478269-02-2P	478269-03-3P	478269-04-4P	478269-05-5P
	478269-06-6P	478269-07-7P	478269-08-8P	478269-09-9P	478269-10-2P
	478269-11-3P	478269-12-4P	478269-13-5P	478269-14-6P	478269-15-7P
	478269-16-8P	478269-17-9P	478269-18-0P	478269-19-1P	478269-20-4P
	478269-21-5P	478269-22-6P	478269-23-7P	478269-24-8P	478269-25-9P
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478269-31-7P	478269-32-8P	478269-33-9P	478269-34-0P	478269-35-1P
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478269-41-9P	478269-42-0P	478269-43-1P	478269-44-2P	478269-45-3P
478269-46-4P	478269-47-5P	478269-48-6P	478269-49-7P	478269-50-0P
478269-51-1P	478269-52-2P	478269-53-3P	478269-54-4P	478269-55-5P
478269-56-6P	478269-57-7P	478269-58-8P	478269-59-9P	478269-60-2P
478269-61-3P	478269-62-4P	478269-63-5P	478269-64-6P	478269-65-7P
478269-66-8P	478269-67-9P	478269-68-0P	478269-69-1P	478269-70-4P
478269-71-5P	478269-72-6P	478269-73-7P	478269-74-8P	478269-75-9P
478269-76-0P	478269-77-1P	478269-78-2P	478269-79-3P	478269-80-6P
478269-81-7P	478269-82-8P	478269-83-9P	478269-84-0P	478269-85-1P
478269-86-2P	478269-87-3P	478269-88-4P	478269-89-5P	478269-90-8P
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478269-96-4P	478269-97-5P	478269-98-6P	478269-99-7P	478270-00-7P
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478271-22-6P	478271-23-7P	478271-24-8P	478271-25-9P	478271-26-0P
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478271-32-8P	478271-33-9P	478271-34-0P	478271-35-1P	478271-36-2P
478271-37-3P	478271-38-4P			

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

IT 478271-39-5P	478271-40-8P	478271-41-9P	478271-42-0P	478271-43-1P
478271-44-2P	478271-45-3P	478271-46-4P	478271-47-5P	478271-48-6P
478271-49-7P	478271-50-0P	478271-51-1P	478271-52-2P	478271-53-3P
478271-54-4P	478271-55-5P	478271-56-6P	478271-57-7P	478271-58-8P
478271-59-9P	478271-60-2P	478271-61-3P	478271-62-4P	478271-63-5P
478271-64-6P	478271-65-7P	478271-66-8P	478271-67-9P	478271-68-0P
478271-69-1P	478271-70-4P	478271-71-5P	478271-72-6P	478271-73-7P
478271-74-8P	478271-75-9P	478271-76-0P	478271-77-1P	478271-78-2P
478271-79-3P	478271-80-6P	478271-81-7P	478271-82-8P	478271-83-9P
478271-84-0P	478271-85-1P	478271-86-2P	478271-87-3P	478271-88-4P
478271-89-5P	478271-90-8P	478271-91-9P	478271-92-0P	478271-93-1P
478271-94-2P	478271-95-3P	478271-96-4P	478271-97-5P	478271-98-6P
478271-99-7P	478272-00-3P	478272-01-4P	478272-02-5P	478272-03-6P
478272-04-7P	478272-05-8P	478272-06-9P	478272-07-0P	478272-08-1P
478272-09-2P	478272-10-5P	478272-11-6P	478272-12-7P	478272-13-8P
478272-14-9P	478272-15-0P	478272-16-1P	478272-17-2P	

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

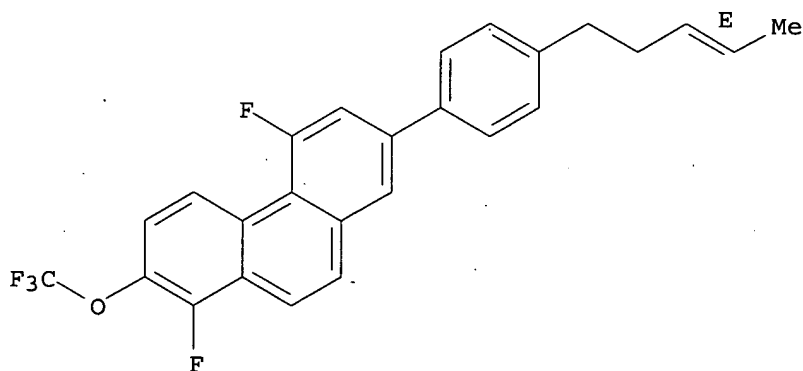
(prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

L6 ANSWER 106 OF 500 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 478269-15-7 REGISTRY
 CN Phenanthrene, 1,5-difluoro-7-[4-(3E)-3-pentenylphenyl]-2-(trifluoromethoxy)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C26 H19 F5 O
 SR CA
 LC STN Files: CA, CAPLUS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1
C6-C6-C6	C6-C6-C6	6-6-6	C14	2404.11.109	1

Double bond geometry as shown.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1000000.0	pH 1	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 4	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 7	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 8	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 10	(1) ACD
Boiling Point (BP)	505.1+/-35.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	74.54+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	269.2+/-39.3 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	5		(1) ACD
H acceptors (HAC)	1		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	3751558	pH 1	(1) ACD
Koc (KOC)	3751558	pH 4	(1) ACD
Koc (KOC)	3751558	pH 7	(1) ACD
Koc (KOC)	3751558	pH 8	(1) ACD
Koc (KOC)	3751558	pH 10	(1) ACD
logD (LOGD)	9.55	pH 1	(1) ACD

logD (LOGD)	9.55	pH 4	(1) ACD
logD (LOGD)	9.55	pH 7	(1) ACD
logD (LOGD)	9.55	pH 8	(1) ACD
logD (LOGD)	9.55	pH 10	(1) ACD
logP (LOGP)	9.554+/-0.753		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	442.42		(1) ACD
Vapor Pressure (VP)	7.87E-10 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

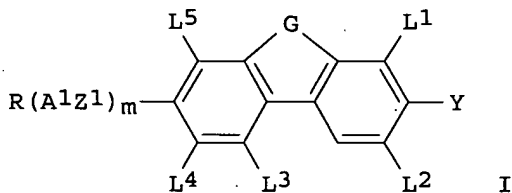
REFERENCE 1

AN 138:31093 CA
TI Fluorinated (dihydro)phenanthrene derivatives and their use in liquid crystalline media
IN Bremer, Matthias; Pauluth, Detlef; Heckmeier, Michael; Duebal, Hans-Rolf; Hornung, Barbara; Schmidt, Wolfgang; Wingen, Rainer
PA Merck Patent G.m.b.H., Germany
SO Ger. Offen., 124 pp.
CODEN: GWXXBX
DT Patent
LA German
IC ICM C07C025-18
ICS C07C025-24; C07C013-62; C07C043-225; C07C069-00; C07C255-00; C07C331-02; C07C331-16; C07C381-00; C09K019-06; G02F001-137; G09F009-35
CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 75

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	DE 10225048	A1	20021212	DE 2002-10225048	20020606
	GB 2377706	A1	20030122	GB 2002-13110	20020607
	JP 2003096003	A2	20030403	JP 2002-166852	20020607
PRAI	DE 2001-10127482		20010607		
	DE 2001-10136965		20010728		

GI



AB The invention relates to a liq. cryst. (dihydro)phenanthrene derivate of the formula I (R = C1-15-alkyl, alkenyl; Al = 1,4-cyclohexenylene, 1,4-cyclohexylene, 1,4-phenylene; Z1 = -COO-, -OCO-, -CF2O-, -OCF2-,

-CH2O-, -OCH2-, -CH2CH2-, -C2F4-, -CH:CH-, -C.tplbond.C-, single bond; Y = H, F, Cl, CN, SF5, NCS, SCN, C1-5-alkyl, alkenyl, alkenyloxy, alkoxy; G = -CH2CH2-, -CH:CF-, -CH:CH-; L1-5 = H, F; m = 0, 1), as well as liq. cryst. media, contg. at least the above (dihydro)phenanthrene deriv., and electrooptical displays contg. the above liq. crystal media. The (dihydro)phenanthrene deriv. were synthesized.

ST fluorinated phenanthrene dihydrophenanthrene synthesis nematic liq crystal mixt display

IT 76802-59-0 76802-61-4 81711-13-9 84540-37-4 84816-56-8
 92263-41-7 94840-77-4 97398-75-9 106349-49-9 116020-44-1
 129738-34-7 131819-23-3 132123-45-6 137528-82-6 138074-20-1
 138981-15-4 139215-80-8 140384-00-5 142400-92-8 151359-01-2
 154346-21-1 155041-85-3 155266-68-5 173837-35-9 173837-36-0
 174805-87-9 181943-55-5 188289-44-3 205806-87-7 247924-91-0
 262604-12-6 262605-14-1 262852-95-9 279246-65-0 288579-85-1
 288579-86-2 315691-10-2 325960-56-3 326894-55-7 440666-89-7
 440666-91-1 478272-37-6 478272-38-7 478272-39-8 478272-40-1
 478272-48-9 478272-49-0 478272-50-3 478272-51-4

RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(liq. crystal mixt. contg. fluorinated (dihydro)phenanthrene derivs. for liq. crystal display)

IT 478264-05-0P 478264-08-3P 478264-19-6P 478265-68-8P 478267-19-5P
 478268-57-4P 478268-76-7P 478270-27-8P 478272-18-3P 478272-19-4P
 478272-20-7P 478272-22-9P 478272-23-0P 478272-24-1P 478272-25-2P
 478272-26-3P 478272-28-5P 478272-29-6P 478272-30-9P 478272-31-0P
 478272-32-1P 478272-33-2P 478272-34-3P 478272-35-4P 478272-36-5P

RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

IT 4009-98-7, Methoxymethyltriphenylphosphoniumchloride 132123-39-8
 RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

IT 478264-03-8P 478264-04-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

IT 478264-06-1P 478264-07-2P 478264-09-4P 478264-10-7P 478264-11-8P
 478264-12-9P 478264-13-0P 478264-14-1P 478264-15-2P 478264-16-3P
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 478264-24-3P 478264-25-4P 478264-26-5P 478264-27-6P 478264-28-7P
 478264-29-8P 478264-30-1P 478264-31-2P 478264-32-3P 478264-33-4P
 478264-34-5P 478264-35-6P 478264-36-7P 478264-37-8P 478264-38-9P
 478264-39-0P 478264-40-3P 478264-41-4P 478264-42-5P 478264-43-6P
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478265-40-6P	478265-41-7P	478265-42-8P	478265-43-9P	478265-44-0P
478265-45-1P	478265-46-2P	478265-47-3P	478265-48-4P	478265-49-5P
478265-50-8P	478265-51-9P	478265-52-0P	478265-53-1P	478265-54-2P
478265-55-3P	478265-56-4P	478265-57-5P	478265-58-6P	478265-59-7P
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478266-36-3P	478266-37-4P	478266-38-5P	478266-39-6P	478266-40-9P
478266-41-0P	478266-42-1P	478266-43-2P	478266-44-3P	478266-45-4P
478266-46-5P	478266-47-6P			

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

IT	478266-48-7P	478266-49-8P	478266-50-1P	478266-51-2P	478266-52-3P
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	478266-58-9P	478266-59-0P	478266-60-3P	478266-61-4P	478266-62-5P
	478266-63-6P	478266-64-7P	478266-65-8P	478266-66-9P	478266-67-0P
	478266-68-1P	478266-69-2P	478266-71-6P	478266-72-7P	478266-73-8P
	478266-74-9P	478266-75-0P	478266-76-1P	478266-77-2P	478266-78-3P
	478266-79-4P	478266-80-7P	478266-81-8P	478266-82-9P	478266-83-0P
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RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
 (prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

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RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
 (prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

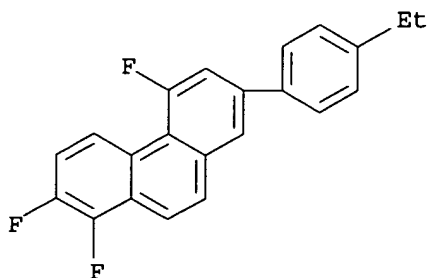
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RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
 (prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

L6 ANSWER 148 OF 500 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 478268-72-3 REGISTRY
 CN Phenanthrene, 7-(4-ethylphenyl)-1,2,5-trifluoro- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C22 H15 F3
 SR CA
 LC STN Files: CA, CAPLUS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
=====	=====	=====	=====	=====	=====
C6	C6	6	C6	46.150.18	1
C6-C6-C6	C6-C6-C6	6-6-6	C14	2404.11.109	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
=====	=====	=====	=====

Bioconc. Factor (BCF)	278879	pH 1	(1) ACD
Bioconc. Factor (BCF)	278879	pH 4	(1) ACD
Bioconc. Factor (BCF)	278879	pH 7	(1) ACD
Bioconc. Factor (BCF)	278879	pH 8	(1) ACD
Bioconc. Factor (BCF)	278879	pH 10	(1) ACD
Boiling Point (BP)	469.1+/-25.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	70.35+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	277.0+/-23.4 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	2		(1) ACD
H acceptors (HAC)	0		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	275045	pH 1	(1) ACD
Koc (KOC)	275045	pH 4	(1) ACD
Koc (KOC)	275045	pH 7	(1) ACD
Koc (KOC)	275045	pH 8	(1) ACD
Koc (KOC)	275045	pH 10	(1) ACD
logD (LOGD)	7.47	pH 1	(1) ACD
logD (LOGD)	7.47	pH 4	(1) ACD
logD (LOGD)	7.47	pH 7	(1) ACD
logD (LOGD)	7.47	pH 8	(1) ACD
logD (LOGD)	7.47	pH 10	(1) ACD
logP (LOGP)	7.468+/-0.529		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	336.35		(1) ACD
Vapor Pressure (VP)	1.59E-08 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

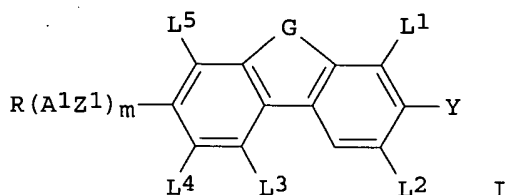
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 138:31093 CA
 TI Fluorinated (dihydro)phenanthrene derivatives and their use in liquid crystalline media
 IN Bremer, Matthias; Pauluth, Detlef; Heckmeier, Michael; Duebal, Hans-Rolf; Hornung, Barbara; Schmidt, Wolfgang; Wingen, Rainer
 PA Merck Patent G.m.b.H., Germany
 SO Ger. Offen., 124 pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 IC ICM C07C025-18
 ICS C07C025-24; C07C013-62; C07C043-225; C07C069-00; C07C255-00; C07C331-02; C07C331-16; C07C381-00; C09K019-06; G02F001-137; G09F009-35
 CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
 Section cross-reference(s): 75
 FAN: CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 10225048	A1	20021212	DE 2002-10225048	20020606
	GB 2377706	A1	20030122	GB 2002-13110	20020607
	JP 2003096003	A2	20030403	JP 2002-166852	20020607
PRAI	DE 2001-10127482		20010607		
	DE 2001-10136965		20010728		

GI



AB The invention relates to a liq. cryst. (dihydro)phenanthrene derivate of the formula I (R = C1-15-alkyl, alkenyl; A1 = 1,4-cyclohexenylene, 1,4-cyclohexylene, 1,4-phenylene; Z1 = -COO-, -OCO-, -CF2O-, -OCF2-, -CH2O-, -OCH2-, -CH2CH2-, -C2F4-, -CH:CH-, -C.tplbond.C-, single bond; Y = H, F, Cl, CN, SF5, NCS, SCN, C1-5-alkyl, alkenyl, alkenyloxy, alkoxy; G = -CH2CH2-, -CH:CF-, -CH:CH-; L1-5 = H, F; m = 0, 1), as well as liq. cryst. media, contg. at least the above (dihydro)phenanthrene deriv., and electrooptical displays contg. the above liq. crystal media. The (dihydro)phenanthrene deriv. were synthesized.

ST fluorinated phenanthrene dihydrophenanthrene synthesis nematic liq crystal mixt display

IT 76802-59-0 76802-61-4 81711-13-9 84540-37-4 84816-56-8
 92263-41-7 94840-77-4 97398-75-9 106349-49-9 116020-44-1
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 138981-15-4 139215-80-8 140384-00-5 142400-92-8 151359-01-2
 154346-21-1 155041-85-3 155266-68-5 173837-35-9 173837-36-0
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RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(liq. crystal mixt. contg. fluorinated (dihydro)phenanthrene derivs. for liq. crystal display)

IT 478264-05-0P 478264-08-3P 478264-19-6P 478265-68-8P 478267-19-5P
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RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

IT 4009-98-7, Methoxymethyltriphenylphosphoniumchloride 132123-39-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

IT 478264-03-8P 478264-04-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

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478265-35-9P	478265-36-0P	478265-37-1P	478265-38-2P	478265-39-3P
478265-40-6P	478265-41-7P	478265-42-8P	478265-43-9P	478265-44-0P
478265-45-1P	478265-46-2P	478265-47-3P	478265-48-4P	478265-49-5P
478265-50-8P	478265-51-9P	478265-52-0P	478265-53-1P	478265-54-2P
478265-55-3P	478265-56-4P	478265-57-5P	478265-58-6P	478265-59-7P
478265-60-0P	478265-61-1P	478265-62-2P	478265-63-3P	478265-64-4P
478265-65-5P	478265-66-6P	478265-67-7P	478265-69-9P	478265-70-2P
478265-71-3P	478265-72-4P	478265-73-5P	478265-74-6P	478265-75-7P
478265-76-8P	478265-77-9P	478265-78-0P	478265-79-1P	478265-80-4P
478265-81-5P	478265-82-6P	478265-83-7P	478265-84-8P	478265-85-9P
478265-86-0P	478265-87-1P	478265-88-2P	478265-89-3P	478265-90-6P
478265-91-7P	478265-92-8P	478265-93-9P	478265-94-0P	478265-95-1P
478265-96-2P	478265-97-3P	478265-98-4P	478265-99-5P	478266-00-1P
478266-01-2P	478266-02-3P	478266-03-4P	478266-04-5P	478266-05-6P
478266-06-7P	478266-07-8P	478266-08-9P	478266-09-0P	478266-10-3P
478266-11-4P	478266-12-5P	478266-13-6P	478266-14-7P	478266-15-8P
478266-16-9P	478266-17-0P	478266-18-1P	478266-19-2P	478266-20-5P
478266-21-6P	478266-22-7P	478266-23-8P	478266-24-9P	478266-25-0P
478266-26-1P	478266-27-2P	478266-28-3P	478266-29-4P	478266-30-7P
478266-31-8P	478266-32-9P	478266-33-0P	478266-34-1P	478266-35-2P
478266-36-3P	478266-37-4P	478266-38-5P	478266-39-6P	478266-40-9P
478266-41-0P	478266-42-1P	478266-43-2P	478266-44-3P	478266-45-4P
478266-46-5P	478266-47-6P			

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

IT	478266-48-7P	478266-49-8P	478266-50-1P	478266-51-2P	478266-52-3P
	478266-53-4P	478266-54-5P	478266-55-6P	478266-56-7P	478266-57-8P
	478266-58-9P	478266-59-0P	478266-60-3P	478266-61-4P	478266-62-5P
	478266-63-6P	478266-64-7P	478266-65-8P	478266-66-9P	478266-67-0P
	478266-68-1P	478266-69-2P	478266-71-6P	478266-72-7P	478266-73-8P
	478266-74-9P	478266-75-0P	478266-76-1P	478266-77-2P	478266-78-3P
	478266-79-4P	478266-80-7P	478266-81-8P	478266-82-9P	478266-83-0P
	478266-84-1P	478266-85-2P	478266-86-3P	478266-87-4P	478266-88-5P
	478266-89-6P	478266-90-9P	478266-91-0P	478266-92-1P	478266-93-2P
	478266-94-3P	478266-95-4P	478266-96-5P	478266-97-6P	478266-98-7P
	478266-99-8P	478267-00-4P	478267-01-5P	478267-02-6P	478267-03-7P
	478267-04-8P	478267-05-9P	478267-06-0P	478267-07-1P	478267-08-2P
	478267-09-3P	478267-10-6P	478267-11-7P	478267-12-8P	478267-13-9P
	478267-14-0P	478267-15-1P	478267-16-2P	478267-17-3P	478267-18-4P
	478267-20-8P	478267-21-9P	478267-22-0P	478267-23-1P	478267-24-2P
	478267-25-3P	478267-26-4P	478267-27-5P	478267-28-6P	478267-29-7P
	478267-30-0P	478267-31-1P	478267-32-2P	478267-33-3P	478267-34-4P
	478267-35-5P	478267-36-6P	478267-37-7P	478267-38-8P	478267-39-9P
	478267-40-2P	478267-41-3P	478267-42-4P	478267-43-5P	478267-44-6P
	478267-45-7P	478267-46-8P	478267-47-9P	478267-48-0P	478267-49-1P
	478267-50-4P	478267-51-5P	478267-52-6P	478267-53-7P	478267-54-8P

478267-55-9P	478267-57-1P	478267-58-2P	478267-59-3P	478267-60-6P
478267-61-7P	478267-62-8P	478267-63-9P	478267-64-0P	478267-65-1P
478267-66-2P	478267-67-3P	478267-68-4P	478267-69-5P	478267-70-8P
478267-71-9P	478267-72-0P	478267-73-1P	478267-74-2P	478267-75-3P
478267-76-4P	478267-77-5P	478267-78-6P	478267-79-7P	478267-80-0P
478267-81-1P	478267-82-2P	478267-83-3P	478267-84-4P	478267-85-5P
478267-86-6P	478267-87-7P	478267-88-8P	478267-89-9P	478267-90-2P
478267-91-3P	478267-92-4P	478267-93-5P	478267-94-6P	478267-95-7P
478267-96-8P	478267-97-9P	478267-98-0P	478267-99-1P	478268-00-7P
478268-01-8P	478268-02-9P	478268-03-0P	478268-04-1P	478268-05-2P
478268-06-3P	478268-07-4P	478268-08-5P	478268-09-6P	478268-10-9P
478268-11-0P	478268-12-1P	478268-13-2P	478268-14-3P	478268-15-4P
478268-16-5P	478268-17-6P	478268-18-7P	478268-19-8P	478268-20-1P
478268-21-2P	478268-22-3P	478268-23-4P	478268-24-5P	478268-25-6P
478268-26-7P	478268-27-8P	478268-28-9P	478268-29-0P	478268-30-3P
478268-31-4P	478268-32-5P	478268-33-6P	478268-34-7P	478268-35-8P
478268-36-9P	478268-37-0P	478268-38-1P	478268-39-2P	478268-40-5P
478268-41-6P	478268-42-7P	478268-43-8P	478268-44-9P	478268-45-0P
478268-46-1P	478268-47-2P	478268-48-3P	478268-49-4P	478268-50-7P
478268-51-8P	478268-52-9P	478268-53-0P	478268-54-1P	478268-55-2P
478268-56-3P	478268-58-5P	478268-59-6P	478268-60-9P	478268-61-0P
478268-62-1P	478268-63-2P	478268-64-3P	478268-65-4P	478268-66-5P
478268-67-6P	478268-68-7P	478268-69-8P	478268-70-1P	478268-71-2P
478268-72-3P	478268-73-4P	478268-74-5P	478268-75-6P	478268-77-8P
478268-78-9P	478268-79-0P	478268-80-3P	478268-81-4P	478268-82-5P
478268-83-6P	478268-84-7P	478268-85-8P	478268-86-9P	478268-87-0P
478268-88-1P	478268-89-2P			

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

IT	478268-90-5P	478268-91-6P	478268-93-8P	478268-94-9P	478268-95-0P
	478268-96-1P	478268-97-2P	478268-98-3P	478268-99-4P	478269-00-0P
	478269-01-1P	478269-02-2P	478269-03-3P	478269-04-4P	478269-05-5P
	478269-06-6P	478269-07-7P	478269-08-8P	478269-09-9P	478269-10-2P
	478269-11-3P	478269-12-4P	478269-13-5P	478269-14-6P	478269-15-7P
	478269-16-8P	478269-17-9P	478269-18-0P	478269-19-1P	478269-20-4P
	478269-21-5P	478269-22-6P	478269-23-7P	478269-24-8P	478269-25-9P
	478269-26-0P	478269-27-1P	478269-28-2P	478269-29-3P	478269-30-6P
	478269-31-7P	478269-32-8P	478269-33-9P	478269-34-0P	478269-35-1P
	478269-36-2P	478269-37-3P	478269-38-4P	478269-39-5P	478269-40-8P
	478269-41-9P	478269-42-0P	478269-43-1P	478269-44-2P	478269-45-3P
	478269-46-4P	478269-47-5P	478269-48-6P	478269-49-7P	478269-50-0P
	478269-51-1P	478269-52-2P	478269-53-3P	478269-54-4P	478269-55-5P
	478269-56-6P	478269-57-7P	478269-58-8P	478269-59-9P	478269-60-2P
	478269-61-3P	478269-62-4P	478269-63-5P	478269-64-6P	478269-65-7P
	478269-66-8P	478269-67-9P	478269-68-0P	478269-69-1P	478269-70-4P
	478269-71-5P	478269-72-6P	478269-73-7P	478269-74-8P	478269-75-9P
	478269-76-0P	478269-77-1P	478269-78-2P	478269-79-3P	478269-80-6P
	478269-81-7P	478269-82-8P	478269-83-9P	478269-84-0P	478269-85-1P
	478269-86-2P	478269-87-3P	478269-88-4P	478269-89-5P	478269-90-8P
	478269-91-9P	478269-92-0P	478269-93-1P	478269-94-2P	478269-95-3P
	478269-96-4P	478269-97-5P	478269-98-6P	478269-99-7P	478270-00-7P
	478270-01-8P	478270-02-9P	478270-03-0P	478270-04-1P	478270-05-2P
	478270-06-3P	478270-07-4P	478270-08-5P	478270-09-6P	478270-10-9P
	478270-11-0P	478270-12-1P	478270-13-2P	478270-14-3P	478270-15-4P
	478270-16-5P	478270-17-6P	478270-18-7P	478270-19-8P	478270-20-1P
	478270-21-2P	478270-22-3P	478270-23-4P	478270-24-5P	478270-25-6P
	478270-26-7P	478270-28-9P	478270-29-0P	478270-30-3P	478270-32-5P
	478270-33-6P	478270-34-7P	478270-35-8P	478270-36-9P	478270-37-0P
	478270-38-1P	478270-39-2P	478270-40-5P	478270-41-6P	478270-42-7P
	478270-43-8P	478270-44-9P	478270-45-0P	478270-46-1P	478270-47-2P
	478270-48-3P	478270-49-4P	478270-50-7P	478270-51-8P	478270-52-9P
	478270-53-0P	478270-54-1P	478270-55-2P	478270-56-3P	478270-57-4P

478270-58-5P	478270-59-6P	478270-60-9P	478270-61-0P	478270-62-1P
478270-63-2P	478270-64-3P	478270-65-4P	478270-66-5P	478270-67-6P
478270-68-7P	478270-69-8P	478270-70-1P	478270-71-2P	478270-72-3P
478270-74-5P	478270-77-8P	478270-78-9P	478270-79-0P	478270-80-3P
478270-81-4P	478270-82-5P	478270-84-7P	478270-85-8P	478270-86-9P
478270-88-1P	478270-90-5P	478270-91-6P	478270-93-8P	478270-94-9P
478270-95-0P	478270-97-2P	478270-99-4P	478271-00-0P	478271-01-1P
478271-02-2P	478271-03-3P	478271-04-4P	478271-05-5P	478271-06-6P
478271-07-7P	478271-08-8P	478271-09-9P	478271-10-2P	478271-11-3P
478271-12-4P	478271-13-5P	478271-14-6P	478271-15-7P	478271-16-8P
478271-17-9P	478271-18-0P	478271-19-1P	478271-20-4P	478271-21-5P
478271-22-6P	478271-23-7P	478271-24-8P	478271-25-9P	478271-26-0P
478271-27-1P	478271-28-2P	478271-29-3P	478271-30-6P	478271-31-7P
478271-32-8P	478271-33-9P	478271-34-0P	478271-35-1P	478271-36-2P
478271-37-3P	478271-38-4P			

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

IT 478271-39-5P	478271-40-8P	478271-41-9P	478271-42-0P	478271-43-1P
478271-44-2P	478271-45-3P	478271-46-4P	478271-47-5P	478271-48-6P
478271-49-7P	478271-50-0P	478271-51-1P	478271-52-2P	478271-53-3P
478271-54-4P	478271-55-5P	478271-56-6P	478271-57-7P	478271-58-8P
478271-59-9P	478271-60-2P	478271-61-3P	478271-62-4P	478271-63-5P
478271-64-6P	478271-65-7P	478271-66-8P	478271-67-9P	478271-68-0P
478271-69-1P	478271-70-4P	478271-71-5P	478271-72-6P	478271-73-7P
478271-74-8P	478271-75-9P	478271-76-0P	478271-77-1P	478271-78-2P
478271-79-3P	478271-80-6P	478271-81-7P	478271-82-8P	478271-83-9P
478271-84-0P	478271-85-1P	478271-86-2P	478271-87-3P	478271-88-4P
478271-89-5P	478271-90-8P	478271-91-9P	478271-92-0P	478271-93-1P
478271-94-2P	478271-95-3P	478271-96-4P	478271-97-5P	478271-98-6P
478271-99-7P	478272-00-3P	478272-01-4P	478272-02-5P	478272-03-6P
478272-04-7P	478272-05-8P	478272-06-9P	478272-07-0P	478272-08-1P
478272-09-2P	478272-10-5P	478272-11-6P	478272-12-7P	478272-13-8P
478272-14-9P	478272-15-0P	478272-16-1P	478272-17-2P	

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

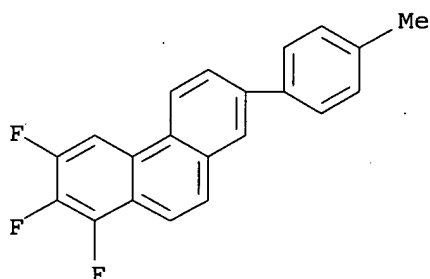
(prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

=> dis 306, 321, 335, 345 all

L6 ANSWER 306 OF 500 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 478267-13-9 REGISTRY
 CN Phenanthrene, 1,2,3-trifluoro-7-(4-methylphenyl)- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C21 H13 F3
 SR CA
 LC STN Files: CA, CAPLUS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1
C6-C6-C6	C6-C6-C6	6-6-6	C14	2404.11.109	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	100478	pH 1	(1) ACD
Bioconc. Factor (BCF)	100478	pH 4	(1) ACD
Bioconc. Factor (BCF)	100478	pH 7	(1) ACD
Bioconc. Factor (BCF)	100478	pH 8	(1) ACD
Bioconc. Factor (BCF)	100478	pH 10	(1) ACD
Boiling Point (BP)	458.9+/-25.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (Hvap)	69.18+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	269.5+/-23.4 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	1		(1) ACD
H acceptors (HAC)	0		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	132453	pH 1	(1) ACD
Koc (KOC)	132453	pH 4	(1) ACD
Koc (KOC)	132453	pH 7	(1) ACD
Koc (KOC)	132453	pH 8	(1) ACD
Koc (KOC)	132453	pH 10	(1) ACD
logD (LOGD)	6.88	pH 1	(1) ACD
logD (LOGD)	6.88	pH 4	(1) ACD
logD (LOGD)	6.88	pH 7	(1) ACD
logD (LOGD)	6.88	pH 8	(1) ACD
logD (LOGD)	6.88	pH 10	(1) ACD
logP (LOGP)	6.884+/-0.520		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	322.32		(1) ACD
Vapor Pressure (VP)	3.60E-08 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

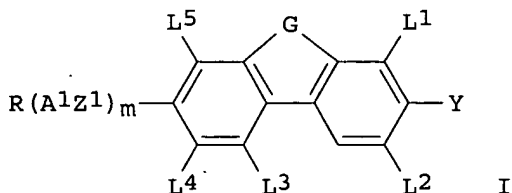
AN 138:31093 CA
TI Fluorinated (dihydro)phenanthrene derivatives and their use in liquid crystalline media
IN Bremer, Matthias; Pauluth, Detlef; Heckmeier, Michael; Duebal, Hans-Rolf; Hornung, Barbara; Schmidt, Wolfgang; Wingen, Rainer
PA Merck Patent G.m.b.H., Germany
SO Ger. Offen., 124 pp.
CODEN: GWXXBX
DT Patent
LA German
IC ICM C07C025-18
ICS C07C025-24; C07C013-62; C07C043-225; C07C069-00; C07C255-00; C07C331-02; C07C331-16; C07C381-00; C09K019-06; G02F001-137; G09F009-35

CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 75

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 10225048	A1	20021212	DE 2002-10225048	20020606
	GB 2377706	A1	20030122	GB 2002-13110	20020607
	JP 2003096003	A2	20030403	JP 2002-166852	20020607
PRAI	DE 2001-10127482		20010607		
	DE 2001-10136965		20010728		

GI



AB The invention relates to a liq. cryst. (dihydro)phenanthrene derivate of the formula I (R = C1-15-alkyl, alkenyl; A1 = 1,4-cyclohexenylene, 1,4-cyclohexylene, 1,4-phenylene; Z1 = -COO-, -OCO-, -CF2O-, -OCF2-, -CH2O-, -OCH2-, -CH2CH2-, -C2F4-, -CH:CH-, -C.tplbond.C-, single bond; Y = H, F, Cl, CN, SF5, NCS, SCN, C1-5-alkyl, alkenyl, alkenyloxy, alkoxy; G = -CH2CH2-, -CH:CF-, -CH:CH-; L1-5 = H, F; m = 0, 1), as well as liq. cryst. media, contg. at least the above (dihydro)phenanthrene deriv., and electrooptical displays contg. the above liq. crystal media. The (dihydro)phenanthrene deriv. were synthesized.

ST fluorinated phenanthrene dihydrophenanthrene synthesis nematic liq crystal mixt display

IT	76802-59-0	76802-61-4	81711-13-9	84540-37-4	84816-56-8
	92263-41-7	94840-77-4	97398-75-9	106349-49-9	116020-44-1
	129738-34-7	131819-23-3	132123-45-6	137528-82-6	138074-20-1
	138981-15-4	139215-80-8	140384-00-5	142400-92-8	151359-01-2
	154346-21-1	155041-85-3	155266-68-5	173837-35-9	173837-36-0
	174805-87-9	181943-55-5	188289-44-3	205806-87-7	247924-91-0
	262604-12-6	262605-14-1	262852-95-9	279246-65-0	288579-85-1
	288579-86-2	315691-10-2	325960-56-3	326894-55-7	440666-89-7
	440666-91-1	478272-37-6	478272-38-7	478272-39-8	478272-40-1
	478272-48-9	478272-49-0	478272-50-3	478272-51-4	

RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(liq. crystal mixt. contg. fluorinated (dihydro)phenanthrene derivs. for liq. crystal display)

IT	478264-05-0P	478264-08-3P	478264-19-6P	478265-68-8P	478267-19-5P
	478268-57-4P	478268-76-7P	478270-27-8P	478272-18-3P	478272-19-4P
	478272-20-7P	478272-22-9P	478272-23-0P	478272-24-1P	478272-25-2P
	478272-26-3P	478272-28-5P	478272-29-6P	478272-30-9P	478272-31-0P
	478272-32-1P	478272-33-2P	478272-34-3P	478272-35-4P	478272-36-5P

RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

IT	4009-98-7, Methoxymethyltriphenylphosphoniumchloride	132123-39-8
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RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

IT	478264-03-8P	478264-04-9P
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

IT	478264-06-1P	478264-07-2P	478264-09-4P	478264-10-7P	478264-11-8P
	478264-12-9P	478264-13-0P	478264-14-1P	478264-15-2P	478264-16-3P
	478264-17-4P	478264-20-9P	478264-21-0P	478264-22-1P	478264-23-2P
	478264-24-3P	478264-25-4P	478264-26-5P	478264-27-6P	478264-28-7P
	478264-29-8P	478264-30-1P	478264-31-2P	478264-32-3P	478264-33-4P
	478264-34-5P	478264-35-6P	478264-36-7P	478264-37-8P	478264-38-9P
	478264-39-0P	478264-40-3P	478264-41-4P	478264-42-5P	478264-43-6P
	478264-44-7P	478264-45-8P	478264-46-9P	478264-47-0P	478264-48-1P
	478264-49-2P	478264-50-5P	478264-51-6P	478264-52-7P	478264-53-8P
	478264-54-9P	478264-55-0P	478264-56-1P	478264-57-2P	478264-58-3P
	478264-59-4P	478264-60-7P	478264-61-8P	478264-62-9P	478264-63-0P
	478264-64-1P	478264-65-2P	478264-66-3P	478264-67-4P	478264-68-5P
	478264-69-6P	478264-70-9P	478264-71-0P	478264-72-1P	478264-73-2P
	478264-74-3P	478264-75-4P	478264-76-5P	478264-77-6P	478264-78-7P
	478264-79-8P	478264-80-1P	478264-81-2P	478264-82-3P	478264-83-4P
	478264-84-5P	478264-85-6P	478264-86-7P	478264-87-8P	478264-88-9P
	478264-89-0P	478264-90-3P	478264-91-4P	478264-92-5P	478264-93-6P
	478264-94-7P	478264-95-8P	478264-96-9P	478264-97-0P	478264-98-1P
	478264-99-2P	478265-00-8P	478265-01-9P	478265-02-0P	478265-03-1P
	478265-04-2P	478265-05-3P	478265-07-5P	478265-08-6P	478265-09-7P
	478265-10-0P	478265-11-1P	478265-12-2P	478265-13-3P	478265-14-4P
	478265-15-5P	478265-16-6P	478265-17-7P	478265-18-8P	478265-19-9P
	478265-20-2P	478265-21-3P	478265-22-4P	478265-23-5P	478265-24-6P
	478265-25-7P	478265-26-8P	478265-27-9P	478265-28-0P	478265-29-1P
	478265-30-4P	478265-31-5P	478265-32-6P	478265-33-7P	478265-34-8P
	478265-35-9P	478265-36-0P	478265-37-1P	478265-38-2P	478265-39-3P
	478265-40-6P	478265-41-7P	478265-42-8P	478265-43-9P	478265-44-0P
	478265-45-1P	478265-46-2P	478265-47-3P	478265-48-4P	478265-49-5P
	478265-50-8P	478265-51-9P	478265-52-0P	478265-53-1P	478265-54-2P
	478265-55-3P	478265-56-4P	478265-57-5P	478265-58-6P	478265-59-7P
	478265-60-0P	478265-61-1P	478265-62-2P	478265-63-3P	478265-64-4P
	478265-65-5P	478265-66-6P	478265-67-7P	478265-69-9P	478265-70-2P

478265-71-3P	478265-72-4P	478265-73-5P	478265-74-6P	478265-75-7P
478265-76-8P	478265-77-9P	478265-78-0P	478265-79-1P	478265-80-4P
478265-81-5P	478265-82-6P	478265-83-7P	478265-84-8P	478265-85-9P
478265-86-0P	478265-87-1P	478265-88-2P	478265-89-3P	478265-90-6P
478265-91-7P	478265-92-8P	478265-93-9P	478265-94-0P	478265-95-1P
478265-96-2P	478265-97-3P	478265-98-4P	478265-99-5P	478266-00-1P
478266-01-2P	478266-02-3P	478266-03-4P	478266-04-5P	478266-05-6P
478266-06-7P	478266-07-8P	478266-08-9P	478266-09-0P	478266-10-3P
478266-11-4P	478266-12-5P	478266-13-6P	478266-14-7P	478266-15-8P
478266-16-9P	478266-17-0P	478266-18-1P	478266-19-2P	478266-20-5P
478266-21-6P	478266-22-7P	478266-23-8P	478266-24-9P	478266-25-0P
478266-26-1P	478266-27-2P	478266-28-3P	478266-29-4P	478266-30-7P
478266-31-8P	478266-32-9P	478266-33-0P	478266-34-1P	478266-35-2P
478266-36-3P	478266-37-4P	478266-38-5P	478266-39-6P	478266-40-9P
478266-41-0P	478266-42-1P	478266-43-2P	478266-44-3P	478266-45-4P
478266-46-5P	478266-47-6P			

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

IT	478266-48-7P	478266-49-8P	478266-50-1P	478266-51-2P	478266-52-3P
	478266-53-4P	478266-54-5P	478266-55-6P	478266-56-7P	478266-57-8P
	478266-58-9P	478266-59-0P	478266-60-3P	478266-61-4P	478266-62-5P
	478266-63-6P	478266-64-7P	478266-65-8P	478266-66-9P	478266-67-0P
	478266-68-1P	478266-69-2P	478266-71-6P	478266-72-7P	478266-73-8P
	478266-74-9P	478266-75-0P	478266-76-1P	478266-77-2P	478266-78-3P
	478266-79-4P	478266-80-7P	478266-81-8P	478266-82-9P	478266-83-0P
	478266-84-1P	478266-85-2P	478266-86-3P	478266-87-4P	478266-88-5P
	478266-89-6P	478266-90-9P	478266-91-0P	478266-92-1P	478266-93-2P
	478266-94-3P	478266-95-4P	478266-96-5P	478266-97-6P	478266-98-7P
	478266-99-8P	478267-00-4P	478267-01-5P	478267-02-6P	478267-03-7P
	478267-04-8P	478267-05-9P	478267-06-0P	478267-07-1P	478267-08-2P
	478267-09-3P	478267-10-6P	478267-11-7P	478267-12-8P	478267-13-9P
	478267-14-0P	478267-15-1P	478267-16-2P	478267-17-3P	478267-18-4P
	478267-20-8P	478267-21-9P	478267-22-0P	478267-23-1P	478267-24-2P
	478267-25-3P	478267-26-4P	478267-27-5P	478267-28-6P	478267-29-7P
	478267-30-0P	478267-31-1P	478267-32-2P	478267-33-3P	478267-34-4P
	478267-35-5P	478267-36-6P	478267-37-7P	478267-38-8P	478267-39-9P
	478267-40-2P	478267-41-3P	478267-42-4P	478267-43-5P	478267-44-6P
	478267-45-7P	478267-46-8P	478267-47-9P	478267-48-0P	478267-49-1P
	478267-50-4P	478267-51-5P	478267-52-6P	478267-53-7P	478267-54-8P
	478267-55-9P	478267-57-1P	478267-58-2P	478267-59-3P	478267-60-6P
	478267-61-7P	478267-62-8P	478267-63-9P	478267-64-0P	478267-65-1P
	478267-66-2P	478267-67-3P	478267-68-4P	478267-69-5P	478267-70-8P
	478267-71-9P	478267-72-0P	478267-73-1P	478267-74-2P	478267-75-3P
	478267-76-4P	478267-77-5P	478267-78-6P	478267-79-7P	478267-80-0P
	478267-81-1P	478267-82-2P	478267-83-3P	478267-84-4P	478267-85-5P
	478267-86-6P	478267-87-7P	478267-88-8P	478267-89-9P	478267-90-2P
	478267-91-3P	478267-92-4P	478267-93-5P	478267-94-6P	478267-95-7P
	478267-96-8P	478267-97-9P	478267-98-0P	478267-99-1P	478268-00-7P
	478268-01-8P	478268-02-9P	478268-03-0P	478268-04-1P	478268-05-2P
	478268-06-3P	478268-07-4P	478268-08-5P	478268-09-6P	478268-10-9P
	478268-11-0P	478268-12-1P	478268-13-2P	478268-14-3P	478268-15-4P
	478268-16-5P	478268-17-6P	478268-18-7P	478268-19-8P	478268-20-1P
	478268-21-2P	478268-22-3P	478268-23-4P	478268-24-5P	478268-25-6P
	478268-26-7P	478268-27-8P	478268-28-9P	478268-29-0P	478268-30-3P
	478268-31-4P	478268-32-5P	478268-33-6P	478268-34-7P	478268-35-8P
	478268-36-9P	478268-37-0P	478268-38-1P	478268-39-2P	478268-40-5P
	478268-41-6P	478268-42-7P	478268-43-8P	478268-44-9P	478268-45-0P
	478268-46-1P	478268-47-2P	478268-48-3P	478268-49-4P	478268-50-7P
	478268-51-8P	478268-52-9P	478268-53-0P	478268-54-1P	478268-55-2P
	478268-56-3P	478268-58-5P	478268-59-6P	478268-60-9P	478268-61-0P
	478268-62-1P	478268-63-2P	478268-64-3P	478268-65-4P	478268-66-5P
	478268-67-6P	478268-68-7P	478268-69-8P	478268-70-1P	478268-71-2P

478268-72-3P	478268-73-4P	478268-74-5P	478268-75-6P	478268-77-8P
478268-78-9P	478268-79-0P	478268-80-3P	478268-81-4P	478268-82-5P
478268-83-6P	478268-84-7P	478268-85-8P	478268-86-9P	478268-87-0P
478268-88-1P	478268-89-2P			

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

IT	478268-90-5P	478268-91-6P	478268-93-8P	478268-94-9P	478268-95-0P
	478268-96-1P	478268-97-2P	478268-98-3P	478268-99-4P	478269-00-0P
	478269-01-1P	478269-02-2P	478269-03-3P	478269-04-4P	478269-05-5P
	478269-06-6P	478269-07-7P	478269-08-8P	478269-09-9P	478269-10-2P
	478269-11-3P	478269-12-4P	478269-13-5P	478269-14-6P	478269-15-7P
	478269-16-8P	478269-17-9P	478269-18-0P	478269-19-1P	478269-20-4P
	478269-21-5P	478269-22-6P	478269-23-7P	478269-24-8P	478269-25-9P
	478269-26-0P	478269-27-1P	478269-28-2P	478269-29-3P	478269-30-6P
	478269-31-7P	478269-32-8P	478269-33-9P	478269-34-0P	478269-35-1P
	478269-36-2P	478269-37-3P	478269-38-4P	478269-39-5P	478269-40-8P
	478269-41-9P	478269-42-0P	478269-43-1P	478269-44-2P	478269-45-3P
	478269-46-4P	478269-47-5P	478269-48-6P	478269-49-7P	478269-50-0P
	478269-51-1P	478269-52-2P	478269-53-3P	478269-54-4P	478269-55-5P
	478269-56-6P	478269-57-7P	478269-58-8P	478269-59-9P	478269-60-2P
	478269-61-3P	478269-62-4P	478269-63-5P	478269-64-6P	478269-65-7P
	478269-66-8P	478269-67-9P	478269-68-0P	478269-69-1P	478269-70-4P
	478269-71-5P	478269-72-6P	478269-73-7P	478269-74-8P	478269-75-9P
	478269-76-0P	478269-77-1P	478269-78-2P	478269-79-3P	478269-80-6P
	478269-81-7P	478269-82-8P	478269-83-9P	478269-84-0P	478269-85-1P
	478269-86-2P	478269-87-3P	478269-88-4P	478269-89-5P	478269-90-8P
	478269-91-9P	478269-92-0P	478269-93-1P	478269-94-2P	478269-95-3P
	478269-96-4P	478269-97-5P	478269-98-6P	478269-99-7P	478270-00-7P
	478270-01-8P	478270-02-9P	478270-03-0P	478270-04-1P	478270-05-2P
	478270-06-3P	478270-07-4P	478270-08-5P	478270-09-6P	478270-10-9P
	478270-11-0P	478270-12-1P	478270-13-2P	478270-14-3P	478270-15-4P
	478270-16-5P	478270-17-6P	478270-18-7P	478270-19-8P	478270-20-1P
	478270-21-2P	478270-22-3P	478270-23-4P	478270-24-5P	478270-25-6P
	478270-26-7P	478270-28-9P	478270-29-0P	478270-30-3P	478270-32-5P
	478270-33-6P	478270-34-7P	478270-35-8P	478270-36-9P	478270-37-0P
	478270-38-1P	478270-39-2P	478270-40-5P	478270-41-6P	478270-42-7P
	478270-43-8P	478270-44-9P	478270-45-0P	478270-46-1P	478270-47-2P
	478270-48-3P	478270-49-4P	478270-50-7P	478270-51-8P	478270-52-9P
	478270-53-0P	478270-54-1P	478270-55-2P	478270-56-3P	478270-57-4P
	478270-58-5P	478270-59-6P	478270-60-9P	478270-61-0P	478270-62-1P
	478270-63-2P	478270-64-3P	478270-65-4P	478270-66-5P	478270-67-6P
	478270-68-7P	478270-69-8P	478270-70-1P	478270-71-2P	478270-72-3P
	478270-74-5P	478270-77-8P	478270-78-9P	478270-79-0P	478270-80-3P
	478270-81-4P	478270-82-5P	478270-84-7P	478270-85-8P	478270-86-9P
	478270-88-1P	478270-90-5P	478270-91-6P	478270-93-8P	478270-94-9P
	478270-95-0P	478270-97-2P	478270-99-4P	478271-00-0P	478271-01-1P
	478271-02-2P	478271-03-3P	478271-04-4P	478271-05-5P	478271-06-6P
	478271-07-7P	478271-08-8P	478271-09-9P	478271-10-2P	478271-11-3P
	478271-12-4P	478271-13-5P	478271-14-6P	478271-15-7P	478271-16-8P
	478271-17-9P	478271-18-0P	478271-19-1P	478271-20-4P	478271-21-5P
	478271-22-6P	478271-23-7P	478271-24-8P	478271-25-9P	478271-26-0P
	478271-27-1P	478271-28-2P	478271-29-3P	478271-30-6P	478271-31-7P
	478271-32-8P	478271-33-9P	478271-34-0P	478271-35-1P	478271-36-2P
	478271-37-3P	478271-38-4P			

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

IT	478271-39-5P	478271-40-8P	478271-41-9P	478271-42-0P	478271-43-1P
	478271-44-2P	478271-45-3P	478271-46-4P	478271-47-5P	478271-48-6P
	478271-49-7P	478271-50-0P	478271-51-1P	478271-52-2P	478271-53-3P
	478271-54-4P	478271-55-5P	478271-56-6P	478271-57-7P	478271-58-8P

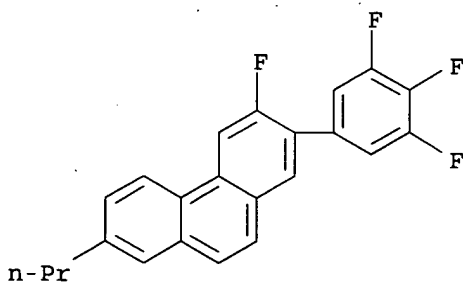
478271-59-9P	478271-60-2P	478271-61-3P	478271-62-4P	478271-63-5P
478271-64-6P	478271-65-7P	478271-66-8P	478271-67-9P	478271-68-0P
478271-69-1P	478271-70-4P	478271-71-5P	478271-72-6P	478271-73-7P
478271-74-8P	478271-75-9P	478271-76-0P	478271-77-1P	478271-78-2P
478271-79-3P	478271-80-6P	478271-81-7P	478271-82-8P	478271-83-9P
478271-84-0P	478271-85-1P	478271-86-2P	478271-87-3P	478271-88-4P
478271-89-5P	478271-90-8P	478271-91-9P	478271-92-0P	478271-93-1P
478271-94-2P	478271-95-3P	478271-96-4P	478271-97-5P	478271-98-6P
478271-99-7P	478272-00-3P	478272-01-4P	478272-02-5P	478272-03-6P
478272-04-7P	478272-05-8P	478272-06-9P	478272-07-0P	478272-08-1P
478272-09-2P	478272-10-5P	478272-11-6P	478272-12-7P	478272-13-8P
478272-14-9P	478272-15-0P	478272-16-1P	478272-17-2P	

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
 (prepn. of fluorinated (dihydro)phenanthrene derivs. for liq. crystal mixt. useful for liq. crystal display)

L6 ANSWER 321 OF 500 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 333737-71-6 REGISTRY
 CN Phenanthrene, 3-fluoro-7-propyl-2-(3,4,5-trifluorophenyl)- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C23 H16 F4
 SR CA
 LC STN Files: CA, CAPLUS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1
C6-C6-C6	C6-C6-C6	6-6-6	C14	2404.11.109	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1351944	pH 1	(1) ACD
Bioconc. Factor (BCF)	1351944	pH 4	(1) ACD
Bioconc. Factor (BCF)	1351944	pH 7	(1) ACD
Bioconc. Factor (BCF)	1351944	pH 8	(1) ACD
Bioconc. Factor (BCF)	1351944	pH 10	(1) ACD
Boiling Point (BP)	470.0+/-25.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	70.44+/-3.0 kJ/mol		(1) ACD

Flash Point (FP)	216.5+/-24.1 deg C		(1) ACD
H acceptors (HAC)	0		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	851348	pH 1	(1) ACD
Koc (KOC)	851348	pH 4	(1) ACD
Koc (KOC)	851348	pH 7	(1) ACD
Koc (KOC)	851348	pH 8	(1) ACD
Koc (KOC)	851348	pH 10	(1) ACD
logD (LOGD)	8.37	pH 1	(1) ACD
logD (LOGD)	8.37	pH 4	(1) ACD
logD (LOGD)	8.37	pH 7	(1) ACD
logD (LOGD)	8.37	pH 8	(1) ACD
logD (LOGD)	8.37	pH 10	(1) ACD
logP (LOGP)	8.370+/-0.573		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	368.37		(1) ACD
Vapor Pressure (VP)	1.49E-08 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

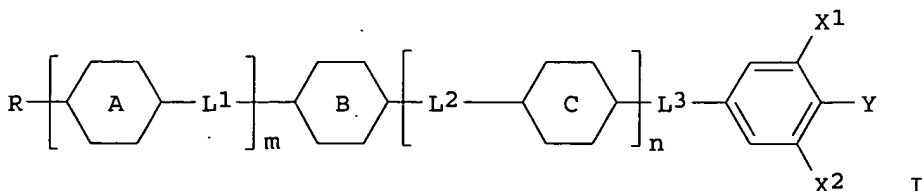
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 134:303137 CA
TI Phenanthrene- or fluorene-containing compounds, their liquid crystal composition, and liquid crystal displays
IN Ogawa, Shinji; Takehara, Sadao; Onishi, Hiroyuki; Takatsu, Haruyoshi
PA Dainippon Ink and Chemicals, Inc., Japan
SO Jpn. Kokai Tokkyo Koho, 81 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
IC ICM C07C025-22
ICS C07C043-225; C07C255-52; C07C255-55; C09K019-32; C09K019-34; G02F001-13
CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 25, 75
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2001106645	A2	20010417	JP 2000-235637	20000803
PRAI	JP 1999-219932		19990803		

GI



AB Cyclocondensation compds. I (R = C1-16 alkyl or alkoxy, C2-16 alkenyl,

C3-16 alkenyloxy, C1-10 alkoxy-substituted C1-12 alkyl; ring A, C = trans-1,4-cyclohexylene, 1,4-phenylene, 1,4-cyclohexenylene, 1,4-bicyclo[2.2.2]octylene, piperidine-1,4-diyl, naphthalene-2,6-diyl, trans-decahydronaphthalene-trans-2,6-diyl, 1,2,3,4-tetrahydronaphthalene-2,6-diyl, their analogs, their derivs.; ring B = (9,10-dihydro)phenanthrene-2,7-diyl, fluorene-2,7-diyl with optional halo substitution; L1-3 = CH₂CH₂, C.tplbond.C, (CH₂)₄, CF:CF, OCH₂, CF₂O, CO₂, CH:NN:CH, CH:CHCH₂CH₂, single bond, etc.; m, n = 0, 1; m + n .ltoreq.1; X1-2 = H, Cl, F; Y = H, F, Cl, tri- or difluoromethoxy, CF₃, 2,2,2-trifluoroethoxy, cyano, C1-12 linear alkyl, C2-12 linear alkenyl, C1-12 linear alkyloxy, etc.) are claimed. Liq. crystal compns. contg. .gtoreq.1 I and liq. crystal displays comprising of the compns. are also claimed. Liq. crystal compns. with wide liq. crystal phase temp. range and decreased threshold voltage are obtained.

ST liq crystal display wide temp operation; phenanthrene deriv liq crystal compn; fluorene deriv liq crystal compn

IT Liquid crystal displays
(liq. crystal compns. contg. (hydro)phenanthrene or fluorene compds. for display devices)

IT 333737-57-8P
RL: DEV (Device component use); IMF (Industrial manufacture); RCT (Reactant); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(liq. crystal compns. contg. (hydro)phenanthrene or fluorene compds. for display devices)

IT 156006-28-9P 326795-64-6P 326795-66-8P 326795-72-6P 326795-73-7P
326795-78-2P 326795-80-6P 326795-82-8P 326795-83-9P 326795-85-1P
326795-86-2P 326795-87-3P 326795-88-4P 326795-90-8P 326795-91-9P
333737-56-7P 333737-71-6P

RL: DEV (Device component use); IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(liq. crystal compns. contg. (hydro)phenanthrene or fluorene compds. for display devices)

IT 40817-08-1D, liq. crystal mixts. contg. 56131-48-7D, liq. crystal mixts. contg. 59855-05-9D, liq. crystal mixts. contg. 61203-99-4D, liq. crystal mixts. contg. 61204-01-1D, liq. crystal mixts. contg. 61204-03-3D, liq. crystal mixts. contg. 67589-39-3D, liq. crystal mixts. contg. 67589-41-7D, liq. crystal mixts. contg. 67589-46-2D, liq. crystal mixts. contg. 67589-47-3D, liq. crystal mixts. contg. 67589-52-0D, liq. crystal mixts. contg. 67589-53-1D, liq. crystal mixts. contg. 67589-69-9D, liq. crystal mixts. contg. 79709-85-6D, liq. crystal mixts. contg. 80944-44-1D, liq. crystal mixts. contg. 86776-52-5D, liq. crystal mixts. contg. 92118-82-6D, liq. crystal mixts. contg. 94412-40-5D, liq. crystal mixts. contg. 95480-29-8D, liq. crystal mixts. contg. 95906-34-6D, liq. crystal mixts. contg. 96184-40-6D, liq. crystal mixts. contg. 96624-52-1D, liq. crystal mixts. contg. 107215-66-7D, liq. crystal mixts. contg. 116903-48-1D, liq. crystal mixts. contg. 118164-50-4D, liq. crystal mixts. contg. 129738-34-7D, liq. crystal mixts. contg. 131819-23-3D, liq. crystal mixts. contg. 132123-39-8D, liq. crystal mixts. contg. 136159-73-4D, liq. crystal mixts. contg. 142400-92-8D, liq. crystal mixts. contg. 145918-41-8D, liq. crystal mixts. contg. 155041-85-3D, liq. crystal mixts. contg. 156243-60-6D, liq. crystal mixts. contg. 184161-94-2D, liq. crystal mixts. contg. 189387-74-4D, liq. crystal mixts. contg. 202652-64-0D, liq. crystal mixts. contg. 284031-60-3D, liq. crystal mixts. contg. 333737-64-7 333737-65-8D, liq. crystal mixts. contg. 333737-66-9 333737-68-1D, liq. crystal mixts. contg.

RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)

(liq. crystal compns. contg. (hydro)phenanthrene or fluorene compds. for display devices)

IT 7506-00-5P 143418-49-9P 157033-24-4P 172366-38-0P 326795-62-4P
326795-63-5P 326795-67-9P 326795-68-0P 326795-69-1P 326795-70-4P
326795-71-5P 326795-74-8P 326795-75-9P 326795-76-0P 326795-77-1P

326795-89-5P 333737-53-4P 333737-54-5P 333737-55-6P 333737-58-9P
 333737-59-0P 333737-60-3P 333737-61-4P 333737-62-5P 333737-73-8P
 RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation);
 RACT (Reactant or reagent)

(liq. crystal compns. contg. (hydro)phenanthrene or fluorene compds.
 for display devices)

IT 79-03-8, Propionic acid chloride 124-41-4, Sodium methoxide 358-23-6,
 Trifluoromethanesulfonic acid anhydride 776-35-2,
 9,10-Dihydrophenanthrene 82380-18-5, 2-Fluoro-4-hydroxybenzonitrile
 105184-38-1, 3,5-Difluorophenylacetic acid 138526-69-9,
 3,4,5-Trifluorobromobenzene 143874-13-9 326795-65-7 326795-79-3
 326795-81-7 333737-63-6

RL: RCT (Reactant); RACT (Reactant or reagent)
 (liq. crystal compns. contg. (hydro)phenanthrene or fluorene compds.
 for display devices)

L6 ANSWER 335 OF 500 REGISTRY COPYRIGHT 2003 ACS on STN

RN 326796-18-3 REGISTRY

CN Phenanthrene, 7-(3,5-difluorophenyl)-8-fluoro-1,2,3,4,4a,9,10,10a-
 octahydro-2-propyl-, (2R,4aS,10aS)-rel- (9CI). (CA INDEX NAME)

FS STEREOSEARCH

MF C23 H25 F3

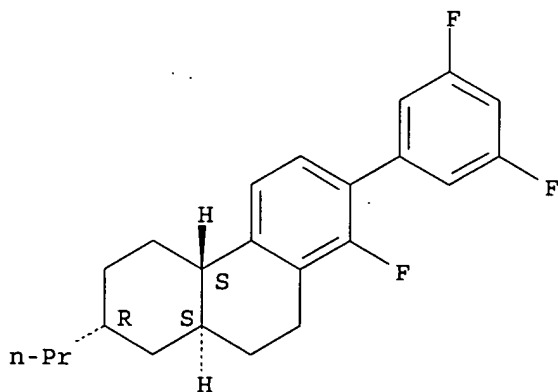
SR CA

LC STN Files: CA, CAPLUS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1
C6-C6-C6	C6-C6-C6	6-6-6	C14	2404.11.58	1

Relative stereochemistry.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	7130694	pH 1	(1) ACD

Bioconc. Factor (BCF)	7130694	pH 4	(1) ACD
Bioconc. Factor (BCF)	7130694	pH 7	(1) ACD
Bioconc. Factor (BCF)	7130694	pH 8	(1) ACD
Bioconc. Factor (BCF)	7130694	pH 10	(1) ACD
Boiling Point (BP)	429.7+/-25.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (Hvap)	65.85+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	248.2+/-23.4 deg C		(1) ACD
H acceptors (HAC)	0		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	2799181	pH 1	(1) ACD
Koc (KOC)	2799181	pH 4	(1) ACD
Koc (KOC)	2799181	pH 7	(1) ACD
Koc (KOC)	2799181	pH 8	(1) ACD
Koc (KOC)	2799181	pH 10	(1) ACD
logD (LOGD)	9.32	pH 1	(1) ACD
logD (LOGD)	9.32	pH 4	(1) ACD
logD (LOGD)	9.32	pH 7	(1) ACD
logD (LOGD)	9.32	pH 8	(1) ACD
logD (LOGD)	9.32	pH 10	(1) ACD
logP (LOGP)	9.320+/-0.531		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	358.44		(1) ACD
Vapor Pressure (VP)	3.45E-07 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

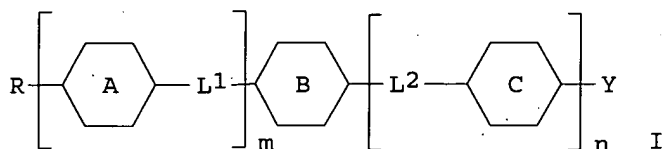
REFERENCE 1

AN 134:186025 CA
 TI Fused ring compound for liquid crystal composition in liquid crystal display device
 IN Ogawa, Shinji; Kawara, Tatsuo; Takehara, Sadao; Ohnishi, Hiroyuki; Takeuchi, Kiyofumi; Takatsu, Haruyoshi; Grahe, Gerwald; Frings, Rainer Bruno; Fugger, Christine; Pithart, Cornelia
 PA Dainippon Ink and Chemicals, Inc., Japan
 SO PCT Int. Appl., 270 pp.
 CODEN: PIXXD2
 DT Patent
 LA Japanese
 IC ICM C07C013-60
 ICS C07C025-22; C07C025-24; C07C039-17; C07C043-225; C07C049-675; C07C255-50; C07C255-55; C09K019-32; C09K019-34; G02F001-13
 CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
 Section cross-reference(s): 75

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001010803	A1	20010215	WO 1999-JP4917	19990910
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK,				

ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG,
 CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
 AU 9956488 A1 20010305 AU 1999-56488 19990910
 EP 1201632 A1 20020502 EP 1999-943249 19990910
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO, MK, CY, AL
 JP 2001106644 A2 20010417 JP 2000-235636 20000803
 PRAI JP 1999-219855 19990803
 WO 1999-JP4917 19990910
 GI



AB The invention relates to a novel compd. I (R = C1-16 alkyl, alkoxy, C2-16 alkenyl, etc.; ring A, C = trans-1,4-cyclohexylene, 1,4-phenylene, 1,4-cyclohexenylene, etc.; ring B = phenantrene deriv., 9H-fluorene deriv.; L1-2 = -CH2CH2-, -CF2=CF2-, -(CH2)4-, etc.; m, n = 0, 1, 2; Y = H, F, Cl, etc.) and a nematic liq. crystal compn. contg. the same. Compd. I can be produced with great ease and has excellent compatibility with a mother liq. crystal of general use being currently used as a nematic liq. crystal, and further shows reduced pptn. at a low temp. The addn. of only a small amt. of compd. I to the mother liq. crystal results in expanding effectively the temp. range for liq. crystallinity, without detriment to various properties as a liq. crystal material. Compd. I is suitable for use in various liq. crystal display elements which are required to have a wide range of metalworking temp. and is greatly useful as a liq. crystal material.

ST fused ring compd liq crystal display device

IT Liquid crystal displays

(fused ring compd. for liq. crystal of liq. crystal display device)

IT Liquid crystals

(nematic; fused ring compd. for liq. crystal of liq. crystal display device)

IT 326795-64-6P 326795-66-8P 326795-72-6P 326795-73-7P 326795-78-2P
 326795-80-6P 326795-82-8P 326795-83-9P 326795-84-0P 326795-85-1P
 326795-86-2P 326795-87-3P 326795-88-4P 326795-90-8P 326795-91-9P
 326795-92-0P 326795-93-1P 326795-94-2P 326795-96-4P 326795-98-6P
 326795-99-7P 326796-03-6P 326796-06-9P 326796-07-0P 326796-10-5P
 326796-11-6P 326796-14-9P 326796-15-0P 326796-16-1P 326796-17-2P
 326796-20-7P 326796-22-9P 326796-24-1P 326796-33-2P 326796-36-5P
 326796-42-3P

RL: DEV (Device component use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(fused ring compd. for liq. crystal of liq. crystal display device)

IT 74-85-1, Ethylene, reactions 78-94-4, Methylvinylketone, reactions
 79-03-8, Propionic acid chloride 79-37-8, Oxalic acid dichloride
 106-38-7, p-Tolyl bromide 110-91-8, Morpholine, reactions 121-43-7,
 Trimethyl borate 124-41-4, Sodium methoxide 624-31-7, p-Iodotoluene
 776-35-2, 9,10-Dihydrophenanthrene 3487-44-3 7664-41-7, Ammonia,
 reactions 10127-56-7, 2,7-Phenanthrenediol 20461-54-5, Iodide,
 reactions 23981-47-7, 6-Methoxy-2-Naphthaleneacetic acid 37865-96-6
 40649-36-3, 4-Propylcyclohexanone 82380-18-5,
 2-Fluoro-4-hydroxybenzonitrile 105184-38-1, 3,5-Difluorophenylacetic
 acid 138526-69-9, 3,4,5-Trifluorobromobenzene 143418-49-9
 143874-13-9 156006-28-9 326795-65-7 326795-79-3 326796-04-7
 326796-18-3 326796-37-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(fused ring compd. for liq. crystal of liq. crystal display device)

IT 927-77-5P, Propylmagnesium bromide 7506-00-5P 82254-81-7P

172366-38-0P	326795-62-4P	326795-63-5P	326795-67-9P	326795-68-0P
326795-69-1P	326795-70-4P	326795-71-5P	326795-74-8P	326795-75-9P
326795-76-0P	326795-77-1P	326795-81-7P	326795-89-5P	326795-95-3P
326795-97-5P	326796-00-3P	326796-01-4P	326796-02-5P	326796-05-8P
326796-08-1P	326796-09-2P	326796-12-7P	326796-13-8P	326796-19-4P
326796-21-8P	326796-23-0P	326796-25-2P	326796-26-3P	326796-27-4P
326796-28-5P	326796-29-6P	326796-30-9P	326796-31-0P	326796-34-3P
326796-35-4P	326796-38-7P	326796-39-8P	326796-40-1P	326796-41-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(fused ring compd. for liq. crystal of liq. crystal display device)

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD

- (1) Canon Inc; JP 05125055 A 1993 CAPLUS
- (2) Canon Inc; JP 05262744 A 1993 CAPLUS
- (3) Chisso Corporation; JP 10236992 1998
- (4) Kabushiki Kaisha Toshiba; JP 2694 A
- (5) Kabushiki Kaisha Toshiba; US 4976887 A CAPLUS
- (6) Kabushiki Kaisha Toshiba; EP 325035 A2 1989 CAPLUS
- (7) Kossmehl, G; Mol Cryst Liq Cryst Sci Technol, Sect A 1995, 269, P39
- (8) Merck Patent Gesellschaft Mit Beschränkter Haftung; DE 3148448 A1 CAPLUS
- (9) Merck Patent Gesellschaft Mit Beschränkter Haftung; JP 58105925 A CAPLUS
- (10) Merck Patent Gesellschaft Mit Beschränkter Haftung; US 4434073 A 1984 CAPLUS

L6 ANSWER 345 OF 500 REGISTRY COPYRIGHT 2003 ACS on STN

RN 326795-98-6 REGISTRY

CN Benzonitrile, 2,6-difluoro-4-[(2R,4aS,4bS,7R,8aS,10aS)-tetradecahydro-7-propyl-2-phenanthrenyl]-, rel- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C24 H31 F2 N

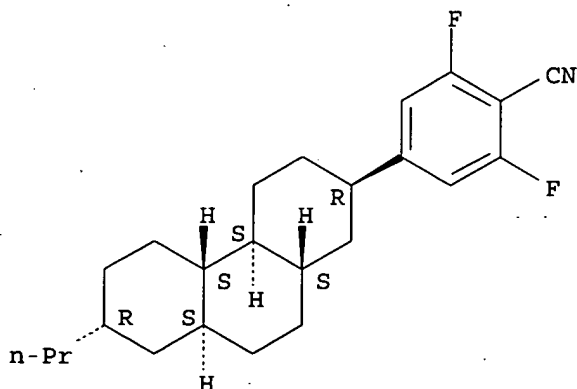
SR CA

LC STN Files: CA, CAPLUS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence Count
EA	ES	SZ	RF	RID	
C6	C6	6	C6	46.150.18	1
C6-C6-C6	C6-C6-C6	6-6-6	C14	2404.11.1	1

Relative stereochemistry.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1796868	pH 1	(1) ACD
Bioconc. Factor (BCF)	1796868	pH 4	(1) ACD
Bioconc. Factor (BCF)	1796868	pH 7	(1) ACD
Bioconc. Factor (BCF)	1796868	pH 8	(1) ACD
Bioconc. Factor (BCF)	1796868	pH 10	(1) ACD
Boiling Point (BP)	457.4+/-30.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	71.75+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	230.4+/-44.2 deg C		(1) ACD
H acceptors (HAC)	1		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	1043635	pH 1	(1) ACD
Koc (KOC)	1043635	pH 4	(1) ACD
Koc (KOC)	1043635	pH 7	(1) ACD
Koc (KOC)	1043635	pH 8	(1) ACD
Koc (KOC)	1043635	pH 10	(1) ACD
logD (LOGD)	8.53	pH 1	(1) ACD
logD (LOGD)	8.53	pH 4	(1) ACD
logD (LOGD)	8.53	pH 7	(1) ACD
logD (LOGD)	8.53	pH 8	(1) ACD
logD (LOGD)	8.53	pH 10	(1) ACD
logP (LOGP)	8.532+/-0.467		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	371.51		(1) ACD
Vapor Pressure (VP)	1.49E-08 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

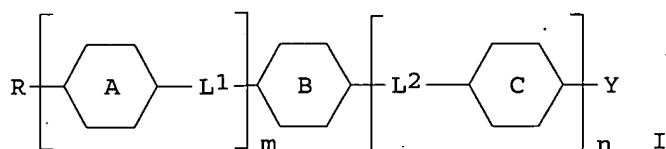
REFERENCE 1

AN 134:186025 CA
TI Fused ring compound for liquid crystal composition in liquid crystal display device
IN Ogawa, Shinji; Kawara, Tatsuo; Takehara, Sadao; Ohnishi, Hiroyuki; Takeuchi, Kiyofumi; Takatsu, Haruyoshi; Grahe, Gerwald; Frings, Rainer Bruno; Fugger, Christine; Pithart, Cornelia
PA Dainippon Ink and Chemicals, Inc., Japan
SO PCT Int. Appl., 270 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
IC ICM C07C013-60
ICS C07C025-22; C07C025-24; C07C039-17; C07C043-225; C07C049-675; C07C255-50; C07C255-55; C09K019-32; C09K019-34; G02F001-13
CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 75

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI WO 2001010803 A1 20010215 WO 1999-JP4917 19990910
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
AU 9956488 A1 20010305 AU 1999-56488 19990910
EP 1201632 A1 20020502 EP 1999-943249 19990910
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL
JP 2001106644 A2 20010417 JP 2000-235636 20000803
PRAI JP 1999-219855 19990803
WO 1999-JP4917 19990910
GI



AB The invention relates to a novel compd. I (R = C1-16 alkyl, alkoxy, C2-16 alkenyl, etc.; ring A, C = trans-1,4-cyclohexylene, 1,4-phenylene, 1,4-cyclohexenylene, etc.; ring B = phenantrene deriv., 9H-fluorene deriv.; L1-2 = -CH2CH2-, -CF2=CF2-, -(CH2)4-, etc.; m, n = 0, 1, 2; Y = H, F, Cl, etc.) and a nematic liq. crystal compn. contg. the same. Compd. I can be produced with great ease and has excellent compatibility with a mother liq. crystal of general use being currently used as a nematic liq. crystal, and further shows reduced pptn. at a low temp. The addn. of only a small amt. of compd. I to the mother liq. crystal results in expanding effectively the temp. range for liq. crystallinity, without detriment to various properties as a liq. crystal material. Compd. I is suitable for use in various liq. crystal display elements which are required to have a wide range of metalworking temp. and is greatly useful as a liq. crystal material.

ST fused ring compd liq crystal display device

IT Liquid crystal displays

(fused ring compd. for liq. crystal of liq. crystal display device)

IT Liquid crystals

(nematic; fused ring compd. for liq. crystal of liq. crystal display device)

IT 326795-64-6P 326795-66-8P 326795-72-6P 326795-73-7P 326795-78-2P
326795-80-6P 326795-82-8P 326795-83-9P 326795-84-0P 326795-85-1P
326795-86-2P 326795-87-3P 326795-88-4P 326795-90-8P 326795-91-9P
326795-92-0P 326795-93-1P 326795-94-2P 326795-96-4P 326795-98-6P
326795-99-7P 326796-03-6P 326796-06-9P 326796-07-0P 326796-10-5P
326796-11-6P 326796-14-9P 326796-15-0P 326796-16-1P 326796-17-2P
326796-20-7P 326796-22-9P 326796-24-1P 326796-33-2P 326796-36-5P
326796-42-3P

RL: DEV (Device component use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(fused ring compd. for liq. crystal of liq. crystal display device)

IT 74-85-1, Ethylene, reactions 78-94-4, Methylvinylketone, reactions
79-03-8, Propionic acid chloride 79-37-8, Oxalic acid dichloride
106-38-7, p-Tolyl bromide 110-91-8, Morpholine, reactions 121-43-7,
Trimethyl borate 124-41-4, Sodium methoxide 624-31-7, p-Iodotoluene

776-35-2, 9,10-Dihydrophenanthrene 3487-44-3 7664-41-7, Ammonia,
 reactions 10127-56-7, 2,7-Phenanthrenediol 20461-54-5, Iodide,
 reactions 23981-47-7, 6-Methoxy-2-Naphthaleneacetic acid 37865-96-6
 40649-36-3, 4-Propylcyclohexanone 82380-18-5,
 2-Fluoro-4-hydroxybenzonitrile 105184-38-1, 3,5-Difluorophenylacetic
 acid 138526-69-9, 3,4,5-Trifluorobromobenzene 143418-49-9
 143874-13-9 156006-28-9 326795-65-7 326795-79-3 326796-04-7
 326796-18-3 326796-37-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(fused ring compd. for liq. crystal of liq. crystal display device)

IT 927-77-5P, Propylmagnesium bromide 7506-00-5P 82254-81-7P
 172366-38-0P 326795-62-4P 326795-63-5P 326795-67-9P 326795-68-0P
 326795-69-1P 326795-70-4P 326795-71-5P 326795-74-8P 326795-75-9P
 326795-76-0P 326795-77-1P 326795-81-7P 326795-89-5P 326795-95-3P
 326795-97-5P 326796-00-3P 326796-01-4P 326796-02-5P 326796-05-8P
 326796-08-1P 326796-09-2P 326796-12-7P 326796-13-8P 326796-19-4P
 326796-21-8P 326796-23-0P 326796-25-2P 326796-26-3P 326796-27-4P
 326796-28-5P 326796-29-6P 326796-30-9P 326796-31-0P 326796-34-3P
 326796-35-4P 326796-38-7P 326796-39-8P 326796-40-1P 326796-41-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(fused ring compd. for liq. crystal of liq. crystal display device)

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD

- (1) Canon Inc; JP 05125055 A 1993 CAPLUS
- (2) Canon Inc; JP 05262744 A 1993 CAPLUS
- (3) Chisso Corporation; JP 10236992 1998
- (4) Kabushiki Kaisha Toshiba; JP 2694 A
- (5) Kabushiki Kaisha Toshiba; US 4976887 A CAPLUS
- (6) Kabushiki Kaisha Toshiba; EP 325035 A2 1989 CAPLUS
- (7) Kossmehl, G; Mol Cryst Liq Cryst Sci Technol, Sect A 1995, 269, P39
- (8) Merck Patent Gesellschaft Mit Beschränkter Haftung; DE 3148448 A1 CAPLUS
- (9) Merck Patent Gesellschaft Mit Beschränkter Haftung; JP 58105925 A CAPLUS
- (10) Merck Patent Gesellschaft Mit Beschränkter Haftung; US 4434073 A 1984
 CAPLUS

(ferroelec.; difluorodihydrophenanthrene derivs. for ferroelec.
liq. crystal mixts. for electrooptical displays)

IT Ferroelectric materials

(liq.-crystal; difluorodihydrophenanthrene derivs.
for ferroelec. liq. crystal mixts. for
electrooptical displays)

IT 209345-87-9P 209345-89-1P 209345-91-5P 209345-93-7P 209345-95-9P
209345-97-1P 209346-00-9P 209346-02-1P 209346-04-3P

RL: SPN (Synthetic preparation); TEM (Technical or engineered material
use); PREP (Preparation); USES (Uses)

(difluorodihydrophenanthrene derivs. for ferroelec. liq.
crystal mixts. for electrooptical displays)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Hoechst Ag; DE 19500768 A 1995 CAPLUS

(2) Hoechst Ag; DE 19517025 A 1996 CAPLUS

(3) Hoechst Ag; DE 19524230 A 1997 CAPLUS

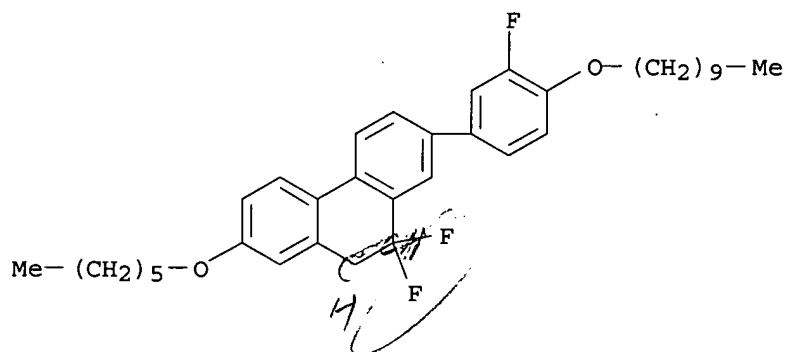
IT 209346-00-9P

RL: SPN (Synthetic preparation); TEM (Technical or engineered material
use); PREP (Preparation); USES (Uses)

(difluorodihydrophenanthrene derivs. for ferroelec. liq.
crystal mixts. for electrooptical displays)

RN 209346-00-9 CAPLUS

CN Phenanthrene, 7-[4-(decyloxy)-3-fluorophenyl]-9,9-difluoro-2-(hexyloxy)-
9,10-dihydro- (9CI) (CA INDEX NAME)

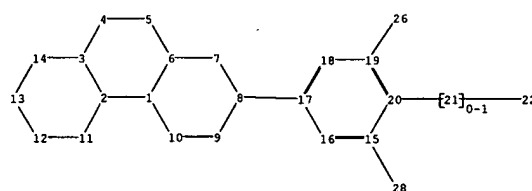
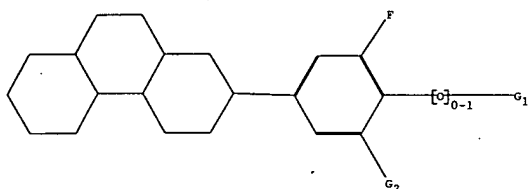


345

3305

321

3006



chain nodes :

21 22 26 28

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

chain bonds :

8-17 15-28 19-26 20-21 21-22

ring bonds :

1-2 1-6 1-10 2-3 2-11 3-4 3-14 4-5 5-6 6-7 7-8 8-9 9-10 11-12 12-13 13-14
15-16 15-20 16-17 17-18 18-19 19-20

exact/norm bonds :

1-2 1-6 1-10 2-3 2-11 3-4 3-14 4-5 5-6 6-7 7-8 8-9 9-10 11-12 12-13 13-14
15-28 20-21 21-22

exact bonds :

8-17 19-26

normalized bonds :

15-16 15-20 16-17 17-18 18-19 19-20

G1:Cl,F,CF2,CF3

G2:H,F

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS
22:CLASS 26:CLASS 28:CLASS

AN 2003:752687 CAPLUS
 DN 139:268384
 TI Preparation of quaterphenyls and related compounds via combinatorial chemistry for use as liquid crystals
 IN Pauluth, Detlef; Kirsch, Peer; Baeuerle, Peter; Deeg, Oliver
 PA Merck Patent G.m.b.H., Germany
 SO Eur. Pat. Appl., 48 pp.
 CODEN: EPXXDW
 DT Patent
 LA German
 IC ICM C07F005-04
 ICS C07C025-18; C09K019-12
 CC 75-8 (Crystallography and Liquid Crystals)
 Section cross-reference(s): 25

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1346995	A1	20030924	EP 2003-3811	20030220
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	DE 10211597	A1	20031002	DE 2002-10211597	20020315
	JP 2003286208	A2	20031010	JP 2003-69260	20030314
PRAI	DE 2002-10211597	A	20020315		
OS	MARPAT 139:268384				
GI					

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I and related compds. [X = single bond, CH₂CH₂, CH=CH, etc.; L = R, halo, OH, etc.; R = alkyl, alkenyl, acylalkyl, etc.; R₁, R₂ = H, F, Cl, etc.] were prepd. For example, Suzuki coupling of terphenyl II, e.g., prepd. from 1,2-difluorobenzene in 5-steps, and boronic acid III afforded quaterphenyl IV in 68% yield. Of note is the use of Suzuki coupling in combinatorial chem.

ST quaterphenyl prepn combinatorial chem suzuki coupling liq crystal

IT Combinatorial chemistry

Liquid crystals

Silylation

Suzuki coupling reaction

(prepn. of quaterphenyls and related compds. via combinatorial chem. for use as liq. crystals)

IT 98-80-6P 54156-71-7P 138871-01-9P 537013-51-7P 574755-30-9P
 574755-40-1P 574755-41-2P 603990-25-6P 603990-27-8P 603990-28-9P
 603990-30-3P 603990-31-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of quaterphenyls and related compds. via combinatorial chem. for use as liq. crystals)

IT 129738-34-7 163185-42-0 477557-80-5 603991-38-4 603991-39-5
 603991-41-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(mixt. contg.; prepn. of quaterphenyls and related compds. via combinatorial chem. for use as liq. crystals)

IT 3375-31-3

RL: CAT (Catalyst use); USES (Uses)

(prepn. of quaterphenyls and related compds. via combinatorial chem. for use as liq. crystals)

IT 67-63-0, Isopropanol, uses 75-05-8, Acetonitrile, uses 123-91-1, Dioxane, uses

RL: NUU (Other use, unclassified); USES (Uses)

(prepn. of quaterphenyls and related compds. via combinatorial chem.)

for use as liq. crystals)

IT 75-77-4, Trimethylsilyl chloride, reactions 121-43-7 126-30-7
 367-11-3, 1,2-Difluorobenzene 461-96-1, 1-Bromo-3,5-difluorobenzene
 534-00-9 624-73-7, 1,2-Diodoethane 2591-86-8, N-Formylpiperidine
 5419-55-6 7790-99-0, Iodine chloride (ICl) 105931-73-5 134150-01-9,
 4-Propylphenylboronic acid 603990-33-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of quaterphenyls and related compds. via combinatorial chem.
 for use as liq. crystals)

IT 603-35-0P, Triphenylphosphine, preparation
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. of quaterphenyls and related compds. via combinatorial chem.
 for use as liq. crystals)

IT 109-72-8, Butyl lithium, reactions 13400-13-0, Cesium fluoride
 17194-00-2, Barium hydroxide
 RL: RGT (Reagent); RACT (Reactant or reagent)
 (prepn. of quaterphenyls and related compds. via combinatorial chem.
 for use as liq. crystals)

IT 603990-35-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of quaterphenyls and related compds. via combinatorial chem.
 for use as liq. crystals)

IT 138220-05-0P 138220-07-2P **326795-86-2P** 478267-19-5P
 478268-76-7P 500001-06-9P 574755-52-5P 574755-53-6P 574755-54-7P
 574755-55-8P 574755-56-9P 574755-59-2P 574755-60-5P 574755-61-6P
 574755-62-7P 574755-63-8P 574755-64-9P 574755-65-0P 574755-66-1P
 574755-67-2P 574755-68-3P 574755-69-4P 574755-70-7P 574755-71-8P
 574755-72-9P 574755-73-0P 574755-74-1P 574755-75-2P 574755-76-3P
 574755-77-4P 574755-78-5P 574755-79-6P 574755-80-9P 574755-81-0P
 574755-82-1P 574755-83-2P 574755-84-3P 574755-85-4P 574755-86-5P
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 603991-11-3P 603991-13-5P 603991-14-6P 603991-15-7P 603991-16-8P
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 603991-23-7P 603991-24-8P 603991-25-9P 603991-26-0P 603991-28-2P
 603991-29-3P 603991-30-6P 603991-31-7P 603991-32-8P 603991-33-9P
 603991-35-1P 603991-36-2P 603991-37-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)

(product; prepn. of quaterphenyls and related compds. via combinatorial chem. for use as liq. crystals)

RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

- (1) Alt, H; J ORGANOMET CHEM 1996
- (2) Anon; PATENT ABSTRACTS OF JAPAN 1996, V1996(07)
- (3) Benneteau, B; TETRAHEDRON 1993, 47
- (4) Chisso Corp; EP 0959060 A 1999 CAPLUS
- (5) Chisso Corp; JP 2002308814 A 2002 CAPLUS
- (6) Coe, P; J.FLUORINE CHEM 1998, 1, CAPLUS
- (7) Deeg, O; CHEMICAL COMMUNICATIONS 2002, 23, P2762 CAPLUS
- (8) Defence Evaluation And Researc; EP 0903391 A 1999 CAPLUS
- (9) Deng, X; J ORG CHEM 2002, 15, CAPLUS
- (10) Frahn, J; SYNTHESIS 1997 CAPLUS
- (11) Hensel, V; EUR J CHEM 1999
- (12) Hensel, V; LIEBIGS ANNALEN/RECEUIL 1997 CAPLUS
- (13) Hird, M; J MATER CHEM 2001
- (14) Hoechst Ag; DE 4426671 A 1996 CAPLUS
- (15) Ici Plc; EP 0470795 A 1992 CAPLUS
- (16) Kaufmann, D; CHEMISCHE BERICHTE 1987, 6, CAPLUS
- (17) Kiryanov, A; JOURNAL OF MATERIALS CHEMISTRY 2001, V11(12), P3068 CAPLUS
- (18) Merck Patent Gmbh; WO 8902425 A 1989 CAPLUS
- (19) Merck Patent Gmbh; WO 9001526 A 1990 CAPLUS
- (20) Merck Patent Gmbh; DE 4220082 A 1993 CAPLUS
- (21) Merck Patent Gmbh; DE 19933175 A 2000 CAPLUS
- (22) Merck Patent Gmbh; GB 2367058 A 2002 CAPLUS
- (23) Seiko Epson Corp; JP 08081416 A 1996 CAPLUS

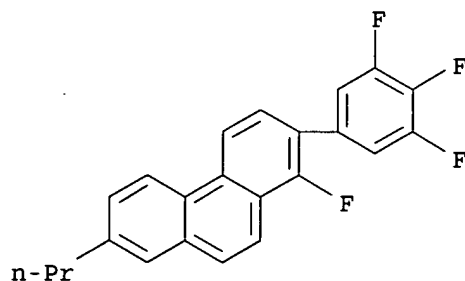
IT 326795-86-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(product; prepn. of quaterphenyls and related compds. via combinatorial chem. for use as liq. crystals)

RN 326795-86-2 CAPLUS

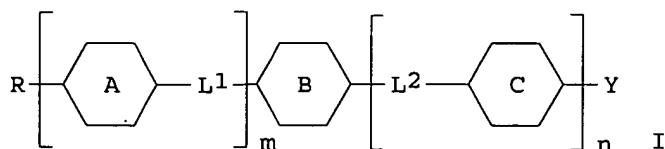
CN Phenanthrene, 1-fluoro-7-propyl-2-(3,4,5-trifluorophenyl)- (9CI) (CA INDEX NAME)



AN 2001:115090 CAPLUS
 DN 134:186025
 TI Fused ring compound for liquid crystal composition in liquid crystal display device
 IN Ogawa, Shinji; Kawara, Tatsuo; Takehara, Sadao; Ohnishi, Hiroyuki; Takeuchi, Kiyofumi; Takatsu, Haruyoshi; Grahe, Gerwald; Frings, Rainer Bruno; Fugger, Christine; Pithart, Cornelia
 PA Dainippon Ink and Chemicals, Inc., Japan
 SO PCT Int. Appl., 270 pp.
 CODEN: PIXXD2
 DT Patent
 LA Japanese
 IC ICM C07C013-60
 ICS C07C025-22; C07C025-24; C07C039-17; C07C043-225; C07C049-675; C07C255-50; C07C255-55; C09K019-32; C09K019-34; G02F001-13
 CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
 Section cross-reference(s): 75

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001010803	A1	20010215	WO 1999-JP4917	19990910
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	AU 9956488	A1	20010305	AU 1999-56488	19990910
	EP 1201632	A1	20020502	EP 1999-943249	19990910
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
	JP 2001106644	A2	20010417	JP 2000-235636	20000803
PRAI	JP 1999-219855	A	19990803		
	WO 1999-JP4917	W	19990910		
OS	MARPAT 134:186025				
GI					



AB The invention relates to a novel compd. I (R = C1-16 alkyl, alkoxy, C2-16 alkenyl, etc.; ring A, C = trans-1,4-cyclohexylene, 1,4-phenylene, 1,4-cyclohexenylene, etc.; ring B = phenantrene deriv., 9H-fluorene deriv.; L1-2 = -CH2CH2-, -CF2=CF2-, -(CH2)4-, etc.; m, n = 0, 1, 2; Y = H, F, Cl, etc.) and a nematic liq. crystal compn. contg. the same. Compd. I can be produced with great ease and has excellent compatibility with a mother liq. crystal of general use being currently used as a nematic liq. crystal, and further shows reduced pptn. at a low temp. The addn. of only a small amt. of compd. I to the mother liq. crystal results in expanding effectively the temp. range for liq. crystallinity, without detriment to various properties as a liq. crystal material. Compd. I is suitable for use in various liq. crystal display elements which are required to have a wide range of metalworking temp. and is greatly useful as a liq. crystal material.

ST fused ring compd liq crystal display device

IT Liquid crystal displays
(fused ring compd. for liq. crystal of liq. crystal display device)

IT Liquid crystals
(nematic; fused ring compd. for liq. crystal of liq. crystal display device)

IT 326795-64-6P 326795-66-8P 326795-72-6P
326795-73-7P 326795-78-2P 326795-80-6P 326795-82-8P
326795-83-9P 326795-84-0P 326795-85-1P 326795-86-2P
326795-87-3P 326795-88-4P 326795-90-8P 326795-91-9P
326795-92-0P 326795-93-1P 326795-94-2P 326795-96-4P
326795-98-6P 326795-99-7P 326796-03-6P 326796-06-9P
326796-07-0P 326796-10-5P 326796-11-6P
326796-14-9P 326796-15-0P 326796-16-1P 326796-17-2P
326796-20-7P 326796-22-9P 326796-24-1P 326796-33-2P 326796-36-5P
326796-42-3P
RL: DEV (Device component use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(fused ring compd. for liq. crystal of liq. crystal display device)

IT 74-85-1, Ethylene, reactions 78-94-4, Methylvinylketone, reactions 79-03-8, Propionic acid chloride 79-37-8, Oxalic acid dichloride 106-38-7, p-Tolyl bromide 110-91-8, Morpholine, reactions 121-43-7, Trimethyl borate 124-41-4, Sodium methoxide 624-31-7, p-Iodotoluene 776-35-2, 9,10-Dihydrophenanthrene 3487-44-3 7664-41-7, Ammonia, reactions 10127-56-7, 2,7-Phenanthrenediol 20461-54-5, Iodide, reactions 23981-47-7, 6-Methoxy-2-Naphthaleneacetic acid 37865-96-6 40649-36-3, 4-Propylcyclohexanone 82380-18-5, 2-Fluoro-4-hydroxybenzonitrile 105184-38-1, 3,5-Difluorophenylacetic acid 138526-69-9, 3,4,5-Trifluorobromobenzene 143418-49-9 143874-13-9 156006-28-9 326795-65-7 326795-79-3 326796-04-7 326796-18-3 326796-37-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(fused ring compd. for liq. crystal of liq. crystal display device)

IT 927-77-5P, Propylmagnesium bromide 7506-00-5P 82254-81-7P
172366-38-0P 326795-62-4P 326795-63-5P 326795-67-9P 326795-68-0P
326795-69-1P 326795-70-4P 326795-71-5P 326795-74-8P 326795-75-9P
326795-76-0P 326795-77-1P 326795-81-7P 326795-89-5P 326795-95-3P
326795-97-5P 326796-00-3P 326796-01-4P 326796-02-5P
326796-05-8P 326796-08-1P 326796-09-2P 326796-12-7P 326796-13-8P
326796-19-4P 326796-21-8P 326796-23-0P 326796-25-2P 326796-26-3P
326796-27-4P 326796-28-5P 326796-29-6P 326796-30-9P 326796-31-0P
326796-34-3P 326796-35-4P 326796-38-7P 326796-39-8P 326796-40-1P
326796-41-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(fused ring compd. for liq. crystal of liq. crystal display device)

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

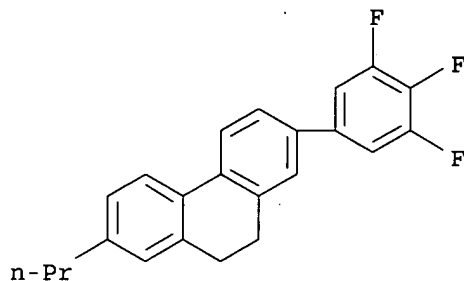
- (1) Canon Inc; JP 05125055 A 1993 CAPLUS
- (2) Canon Inc; JP 05262744 A 1993 CAPLUS
- (3) Chisso Corporation; JP 10236992 1998
- (4) Kabushiki Kaisha Toshiba; JP 2694 A
- (5) Kabushiki Kaisha Toshiba; US 4976887 A CAPLUS
- (6) Kabushiki Kaisha Toshiba; EP 325035 A2 1989 CAPLUS
- (7) Kossmehl, G; Mol Cryst Liq Cryst Sci Technol, Sect A 1995, 269, P39
- (8) Merck Patent Gesellschaft Mit Beschränkter Haftung; DE 3148448 A1 CAPLUS
- (9) Merck Patent Gesellschaft Mit Beschränkter Haftung; JP 58105925 A CAPLUS
- (10) Merck Patent Gesellschaft Mit Beschränkter Haftung; US 4434073 A 1984 CAPLUS

IT 326795-64-6P 326795-72-6P 326795-73-7P
326795-78-2P 326795-84-0P 326795-86-2P
326795-92-0P 326795-94-2P 326796-03-6P
326796-06-9P 326796-10-5P 326796-11-6P
326796-14-9P

RL: DEV (Device component use); SPN (Synthetic preparation); PREP
(Preparation); USES (Uses)
(fused ring compd. for liq. crystal of liq. crystal display device)

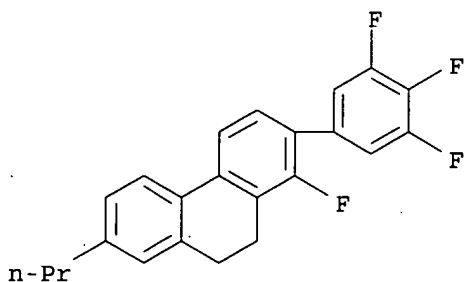
RN 326795-64-6 CAPLUS

CN Phenanthrene, 9,10-dihydro-2-propyl-7-(3,4,5-trifluorophenyl)- (9CI) (CA
INDEX NAME)



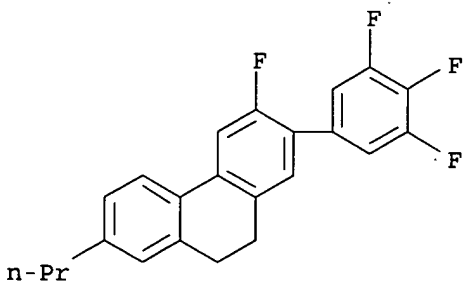
RN 326795-72-6 CAPLUS

CN Phenanthrene, 1-fluoro-9,10-dihydro-7-propyl-2-(3,4,5-trifluorophenyl)-
(9CI) (CA INDEX NAME)



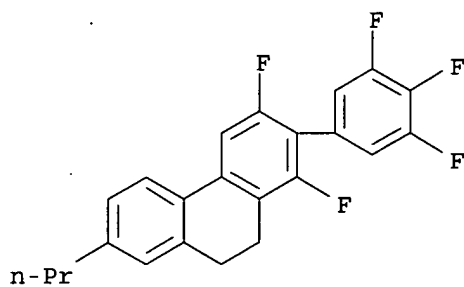
RN 326795-73-7 CAPLUS

CN Phenanthrene, 3-fluoro-9,10-dihydro-7-propyl-2-(3,4,5-trifluorophenyl)-
(9CI) (CA INDEX NAME)

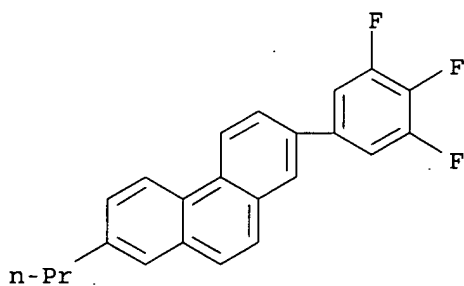


RN 326795-78-2 CAPLUS

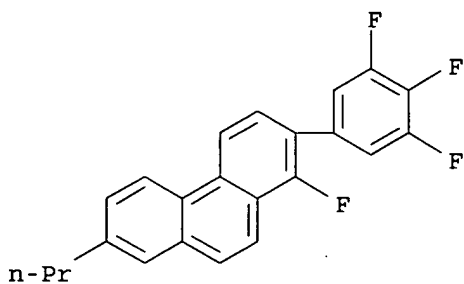
CN Phenanthrene, 1,3-difluoro-9,10-dihydro-7-propyl-2-(3,4,5-trifluorophenyl)-
(9CI) (CA INDEX NAME)



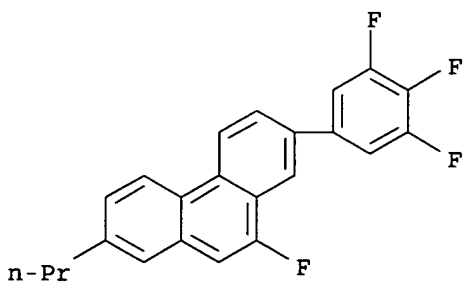
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 CN Phenanthrene, 2-propyl-7-(3,4,5-trifluorophenyl)- (9CI) (CA INDEX NAME)



RN 326795-86-2 CAPLUS
 CN Phenanthrene, 1-fluoro-7-propyl-2-(3,4,5-trifluorophenyl)- (9CI) (CA INDEX NAME)



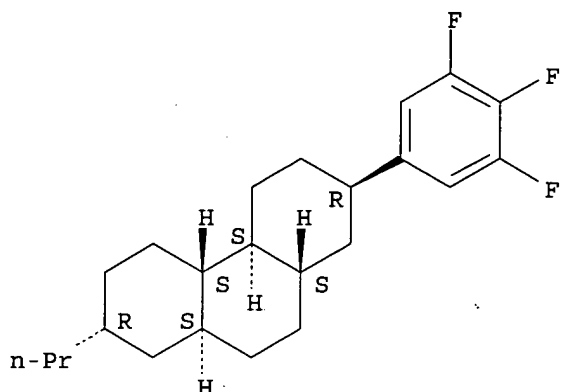
RN 326795-92-0 CAPLUS
 CN Phenanthrene, 9-fluoro-2-propyl-7-(3,4,5-trifluorophenyl)- (9CI) (CA INDEX NAME)



RN 326795-94-2 CAPLUS
 CN Phenanthrene, tetradecahydro-2-propyl-7-(3,4,5-trifluorophenyl)-,

(2R,4aS,4bS,7R,8aS,10aS)-rel- (9CI) (CA INDEX NAME)

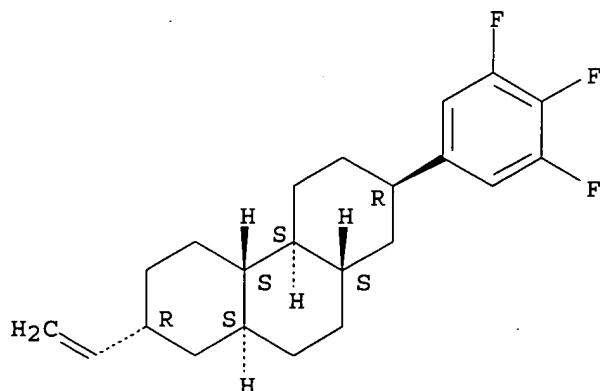
Relative stereochemistry.



RN 326796-03-6 CAPLUS

CN Phenanthrene, 2-ethenyltetradecahydro-7-(3,4,5-trifluorophenyl)-,
(2R,4aS,4bS,7R,8aS,10aS)-rel- (9CI) (CA INDEX NAME)

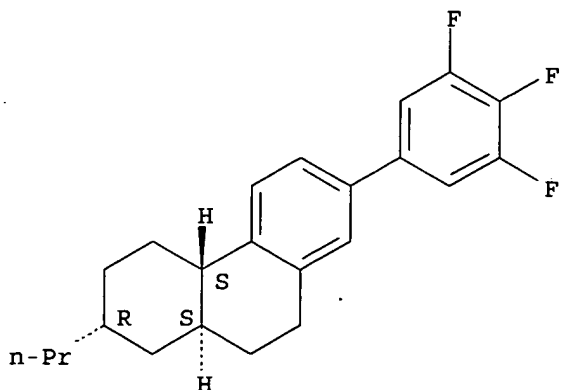
Relative stereochemistry.



RN 326796-06-9 CAPLUS

CN Phenanthrene, 1,2,3,4,4a,9,10,10a-octahydro-2-propyl-7-(3,4,5-trifluorophenyl)-, (2R,4aS,10aS)-rel- (9CI) (CA INDEX NAME)

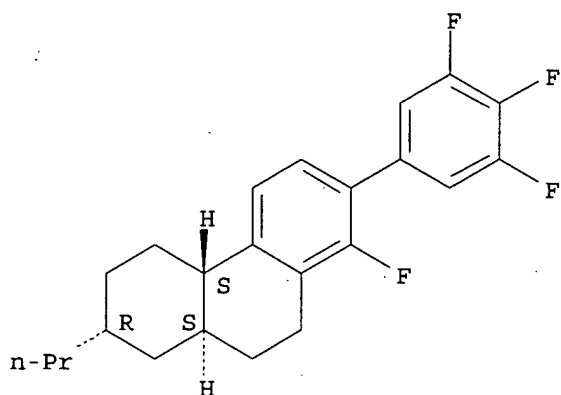
Relative stereochemistry.



RN 326796-10-5 CAPLUS

CN Phenanthrene, 8-fluoro-1,2,3,4,4a,9,10,10a-octahydro-2-propyl-7-(3,4,5-trifluorophenyl)-, (2R,4aS,10aS)-rel- (9CI) (CA INDEX NAME)

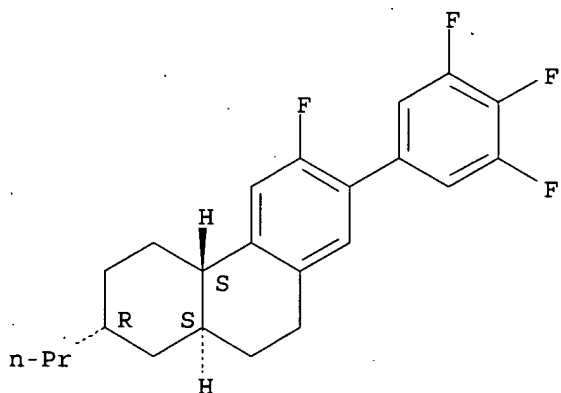
Relative stereochemistry.



RN 326796-11-6 CAPLUS

CN Phenanthrene, 6-fluoro-1,2,3,4,4a,9,10,10a-octahydro-2-propyl-7-(3,4,5-trifluorophenyl)-, (2R,4aS,10aS)-rel- (9CI) (CA INDEX NAME)

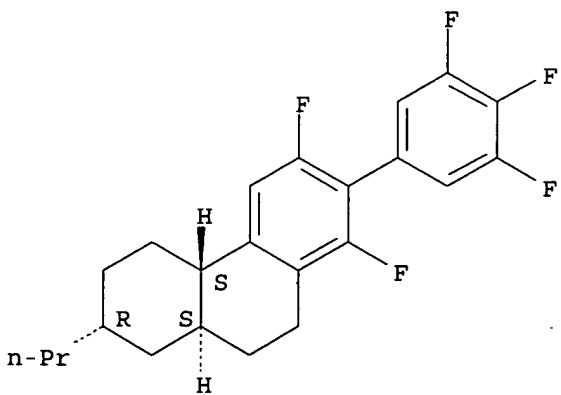
Relative stereochemistry.

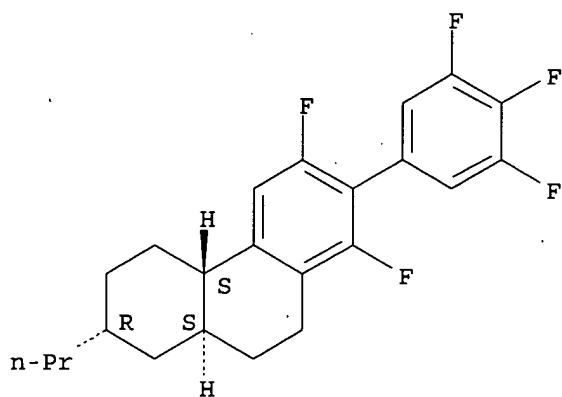


RN 326796-14-9 CAPLUS

CN Phenanthrene, 6,8-difluoro-1,2,3,4,4a,9,10,10a-octahydro-2-propyl-7-(3,4,5-trifluorophenyl)-, (2R,4aS,10aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.





IT 326796-01-4P 326796-02-5P

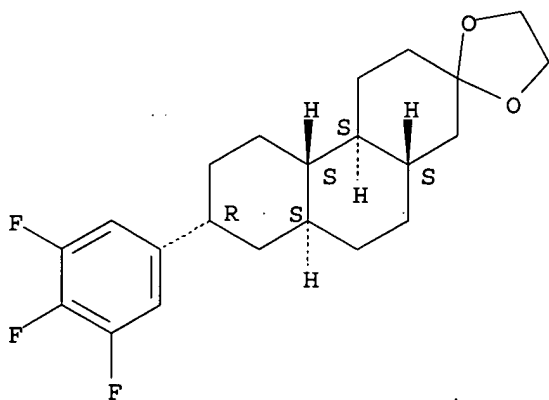
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(fused ring compd. for liq. crystal of liq. crystal display device)

RN 326796-01-4 CAPLUS

CN Spiro[1,3-dioxolane-2,2'-(1'H)-phenanthrene], dodecahydro-7'-(3,4,5-trifluorophenyl)-, (4'aR,4'bR,7'S,8'aR,10'aR)-rel- (9CI) (CA INDEX NAME)

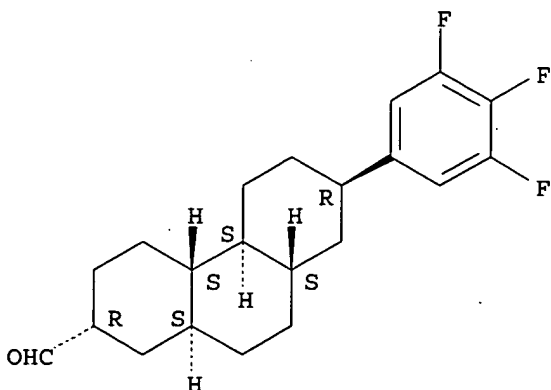
Relative stereochemistry.



RN 326796-02-5 CAPLUS

CN 2-Phenanthrenecarboxaldehyde, tetradecahydro-7-(3,4,5-trifluorophenyl)-, (2R,4aS,4bS,7R,8aS,10aS)-rel- (9CI) (CA INDEX NAME)

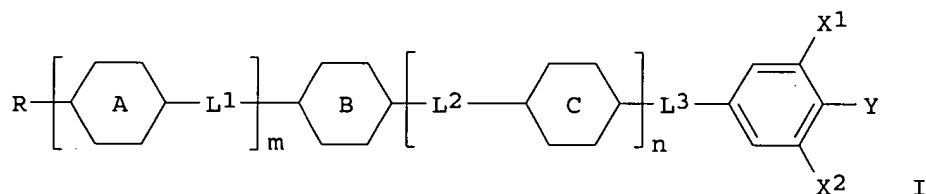
Relative stereochemistry.



AN 2001:270405 CAPLUS
 DN 134:303137
 TI Phenanthrene- or fluorene-containing compounds, their liquid crystal composition, and liquid crystal displays
 IN Ogawa, Shinji; Takehara, Sadao; Onishi, Hiroyuki; Takatsu, Haruyoshi
 PA Dainippon Ink and Chemicals, Inc., Japan
 SO Jpn. Kokai Tokkyo Koho, 81 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 IC ICM C07C025-22
 ICS C07C043-225; C07C255-52; C07C255-55; C09K019-32; C09K019-34; G02F001-13
 CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
 Section cross-reference(s): 25, 75

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2001106645	A2	20010417	JP 2000-235637	20000803
PRAI	JP 1999-219932	A	19990803		
OS	MARPAT 134:303137				
GI					



AB Cyclocondensation compds. I (R = C1-16 alkyl or alkoxy, C2-16 alkenyl, C3-16 alkenyloxy, C1-10 alkoxy-substituted C1-12 alkyl; ring A, C = trans-1,4-cyclohexylene, 1,4-phenylene, 1,4-cyclohexenylene, 1,4-bicyclo[2.2.2]octylene, piperidine-1,4-diyl, naphthalene-2,6-diyl, trans-decahydronaphthalene-trans-2,6-diyl, 1,2,3,4-tetrahydronaphthalene-2,6-diyl, their analogs, their derivs.; ring B = (9,10-dihydro)phenanthrene-2,7-diyl, fluorene-2,7-diyl with optional halo substitution; L1-3 = CH₂CH₂, C.tplbond.C, (CH₂)₄, CF:CF, OCH₂, CF₂O, CO₂, CH:NN:CH, CH:CHCH₂CH₂, single bond, etc.; m, n = 0, 1; m + n .ltoreq.1; X1-2 = H, Cl, F; Y = H, F, Cl, tri- or difluoromethoxy, CF₃, 2,2,2-trifluoroethoxy, cyano, C1-12 linear alkyl, C2-12 linear alkenyl, C1-12 linear alkyloxy, etc.) are claimed. Liq. crystal compns. contg. .gtoreq.1 I and liq. crystal displays comprising of the compns. are also claimed. Liq. crystal compns. with wide liq. crystal phase temp. range and decreased threshold voltage are obtained.

ST liq crystal display wide temp operation; phenanthrene deriv liq crystal compn; fluorene deriv liq crystal compn

IT Liquid crystal displays
 (liq. crystal compns. contg. (hydro)phenanthrene or fluorene compds. for display devices)

IT 333737-57-8P
 RL: DEV (Device component use); IMF (Industrial manufacture); RCT (Reactant); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (liq. crystal compns. contg. (hydro)phenanthrene or fluorene compds. for display devices)

IT 156006-28-9P 326795-64-6P 326795-66-8P 326795-72-6P
 326795-73-7P 326795-78-2P 326795-80-6P 326795-82-8P
 326795-83-9P 326795-85-1P 326795-86-2P 326795-87-3P

326795-88-4P 326795-90-8P 326795-91-9P 333737-56-7P

333737-71-6P

RL: DEV (Device component use); IMF (Industrial manufacture); TEM
(Technical or engineered material use); PREP (Preparation); USES (Uses)
(liq. crystal compns. contg. (hydro)phenanthrene or fluorene compds.
for display devices)

IT 40817-08-1D, liq. crystal mixts. contg. 56131-48-7D, liq. crystal mixts.
contg. 59855-05-9D, liq. crystal mixts. contg. 61203-99-4D, liq.
crystal mixts. contg. 61204-01-1D, liq. crystal mixts. contg.
61204-03-3D, liq. crystal mixts. contg. 67589-39-3D, liq. crystal mixts.
contg. 67589-41-7D, liq. crystal mixts. contg. 67589-46-2D, liq.
crystal mixts. contg. 67589-47-3D, liq. crystal mixts. contg.
67589-52-0D, liq. crystal mixts. contg. 67589-53-1D, liq. crystal mixts.
contg. 67589-69-9D, liq. crystal mixts. contg. 79709-85-6D, liq.
crystal mixts. contg. 80944-44-1D, liq. crystal mixts. contg.
86776-52-5D, liq. crystal mixts. contg. 92118-82-6D, liq. crystal mixts.
contg. 94412-40-5D, liq. crystal mixts. contg. 95480-29-8D, liq.
crystal mixts. contg. 95906-34-6D, liq. crystal mixts. contg.
96184-40-6D, liq. crystal mixts. contg. 96624-52-1D, liq. crystal mixts.
contg. 107215-66-7D, liq. crystal mixts. contg. 116903-48-1D, liq.
crystal mixts. contg. 118164-50-4D, liq. crystal mixts. contg.
129738-34-7D, liq. crystal mixts. contg. 131819-23-3D, liq. crystal
mixts. contg. 132123-39-8D, liq. crystal mixts. contg. 136159-73-4D,
liq. crystal mixts. contg. 142400-92-8D, liq. crystal mixts. contg.
145918-41-8D, liq. crystal mixts. contg. 155041-85-3D, liq. crystal
mixts. contg. 156243-60-6D, liq. crystal mixts. contg. 184161-94-2D,
liq. crystal mixts. contg. 189387-74-4D, liq. crystal mixts. contg.
202652-64-0D, liq. crystal mixts. contg. 284031-60-3D, liq. crystal
mixts. contg. 333737-64-7 333737-65-8D, liq. crystal mixts.
contg. 333737-66-9 333737-68-1D, liq. crystal mixts. contg.

RL: DEV (Device component use); TEM (Technical or engineered material
use); USES (Uses)

(liq. crystal compns. contg. (hydro)phenanthrene or fluorene compds.
for display devices)

IT 7506-00-5P 143418-49-9P 157033-24-4P 172366-38-0P 326795-62-4P
326795-63-5P 326795-67-9P 326795-68-0P 326795-69-1P 326795-70-4P
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326795-89-5P 333737-53-4P 333737-54-5P 333737-55-6P 333737-58-9P
333737-59-0P 333737-60-3P 333737-61-4P 333737-62-5P 333737-73-8P

RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation);
RACT (Reactant or reagent)

(liq. crystal compns. contg. (hydro)phenanthrene or fluorene compds.
for display devices)

IT 79-03-8, Propionic acid chloride 124-41-4, Sodium methoxide 358-23-6,
Trifluoromethanesulfonic acid anhydride 776-35-2, 9,10-
Dihydrophenanthrene 82380-18-5, 2-Fluoro-4-hydroxybenzonitrile
105184-38-1, 3,5-Difluorophenylacetic acid 138526-69-9,
3,4,5-Trifluorobromobenzene 143874-13-9 326795-65-7 326795-79-3
326795-81-7 333737-63-6

RL: RCT (Reactant); RACT (Reactant or reagent)

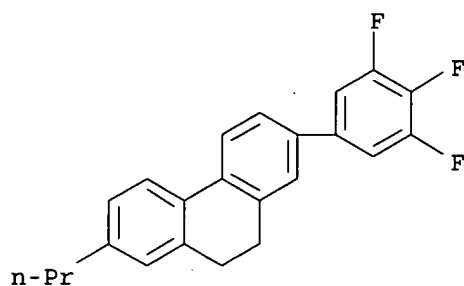
(liq. crystal compns. contg. (hydro)phenanthrene or fluorene compds.
for display devices)

IT 326795-64-6P 326795-72-6P 326795-73-7P
326795-78-2P 326795-86-2P 333737-71-6P

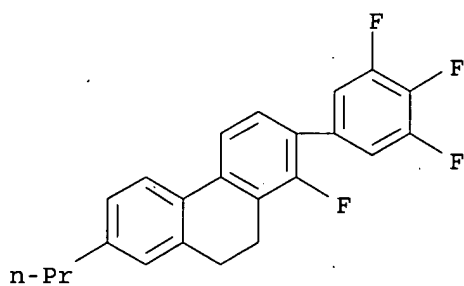
RL: DEV (Device component use); IMF (Industrial manufacture); TEM
(Technical or engineered material use); PREP (Preparation); USES (Uses)
(liq. crystal compns. contg. (hydro)phenanthrene or fluorene compds.
for display devices)

RN 326795-64-6 CAPLUS

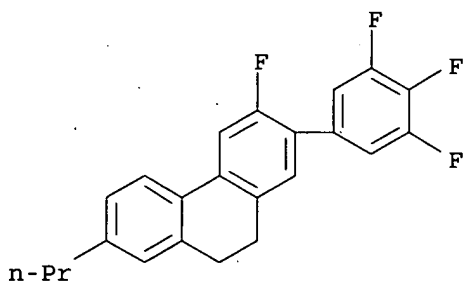
CN Phenanthrene, 9,10-dihydro-2-propyl-7-(3,4,5-trifluorophenyl)- (9CI) (CA
INDEX NAME)



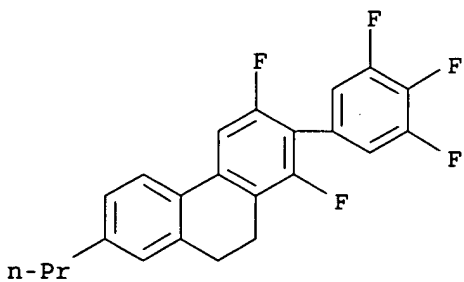
RN 326795-72-6 CAPLUS
 CN Phenanthrene, 1-fluoro-9,10-dihydro-7-propyl-2-(3,4,5-trifluorophenyl)-
 (9CI) (CA INDEX NAME)



RN 326795-73-7 CAPLUS
 CN Phenanthrene, 3-fluoro-9,10-dihydro-7-propyl-2-(3,4,5-trifluorophenyl)-
 (9CI) (CA INDEX NAME)

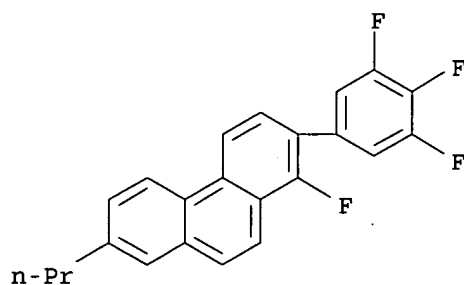


RN 326795-78-2 CAPLUS
 CN Phenanthrene, 1,3-difluoro-9,10-dihydro-7-propyl-2-(3,4,5-trifluorophenyl)-
 (9CI) (CA INDEX NAME)



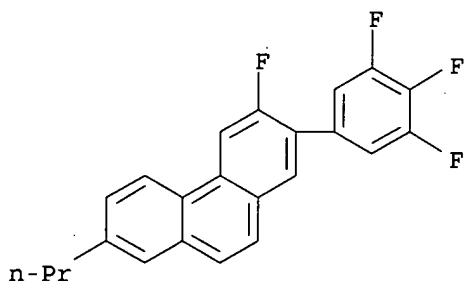
RN 326795-86-2 CAPLUS

CN Phenanthrene, 1-fluoro-7-propyl-2-(3,4,5-trifluorophenyl)- (9CI) (CA INDEX NAME)



RN 333737-71-6 CAPLUS

CN Phenanthrene, 3-fluoro-7-propyl-2-(3,4,5-trifluorophenyl)- (9CI) (CA INDEX NAME)



IT 333737-64-7

RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)

(liq. crystal compns. contg. (hydro)phenanthrene or fluorene compds. for display devices)

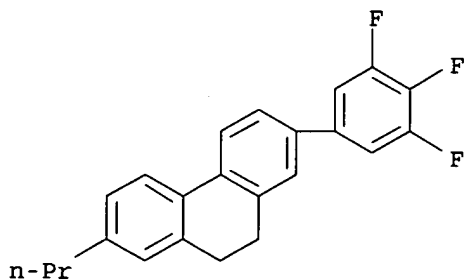
RN 333737-64-7 CAPLUS

CN Phenanthrene, 9,10-dihydro-2-propyl-7-(3,4,5-trifluorophenyl)-, mixt. with 4-[(trans,trans)-4'-(3-butenyl)[1,1'-bicyclohexyl]-4-yl]-1,2-difluorobenzene and 4-[(trans,trans)-4'-ethenyl[1,1'-bicyclohexyl]-4-yl]-1,2-difluorobenzene (9CI) (CA INDEX NAME)

CM 1

CRN 326795-64-6

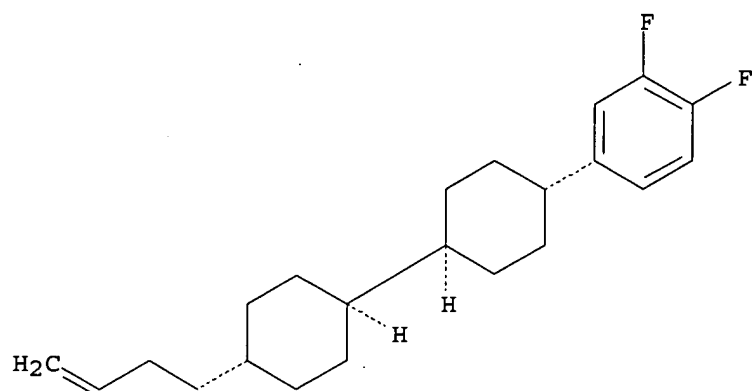
CMF C23 H19 F3



CM 2

CRN 155266-68-5
CMF C22 H30 F2

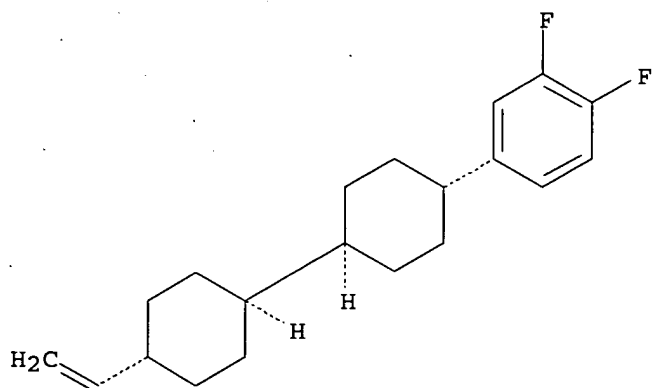
Relative stereochemistry.

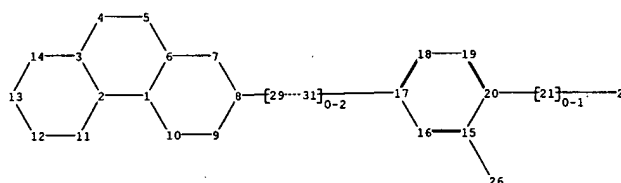
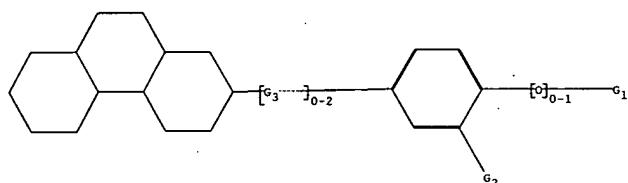


CM 3

CRN 142400-92-8
CMF C20 H26 F2

Relative stereochemistry.





chain nodes :

21 22 26 29 31

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

chain bonds :

8-29 15-26 17-31 20-21 21-22 29-31

ring bonds :

1-2 1-6 1-10 2-3 2-11 3-4 3-14 4-5 5-6 6-7 7-8 8-9 9-10 11-12 12-13 13-14
15-16 15-20 16-17 17-18 18-19 19-20

exact/norm bonds :

1-2 1-6 1-10 2-3 2-11 3-4 3-14 4-5 5-6 6-7 7-8 8-9 8-29 9-10 11-12 12-13
13-14 15-26 20-21 21-22 29-31

exact bonds :

17-31

normalized bonds :

15-16 15-20 16-17 17-18 18-19 19-20

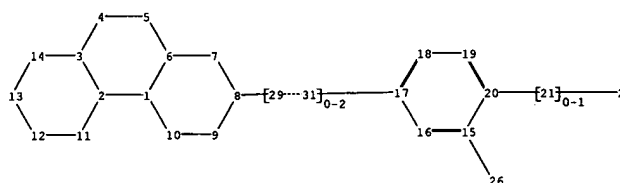
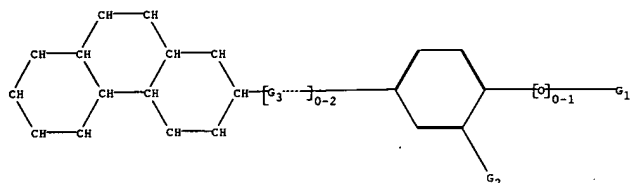
G1:Cl,F,CF2,CF3,C,H,O,CH3,Et,n-Pr,CN

G2:H,F

G3:C,O

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS
22:CLASS 26:CLASS 29:CLASS 31:CLASS



chain nodes :

21 22 26 29 31

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

chain bonds :

8-29 15-26 17-31 20-21 21-22 29-31

ring bonds :

1-2 1-6 1-10 2-3 2-11 3-4 3-14 4-5 5-6 6-7 7-8 8-9 9-10 11-12 12-13 13-14
15-16 15-20 16-17 17-18 18-19 19-20

exact/norm bonds :

1-2 1-6 1-10 2-3 2-11 3-4 3-14 4-5 5-6 6-7 7-8 8-9 8-29 9-10 11-12 12-13
13-14 15-26 20-21 21-22 29-31

exact bonds :

17-31

normalized bonds :

15-16 15-20 16-17 17-18 18-19 19-20

G1:Cl,F,CF2,CF3,C,H,O,CH3,Et,n-Pr,CN

G2:H,F

G3:C,O

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS
22:CLASS 26:CLASS 29:CLASS 31:CLASS

(FILE 'HOME' ENTERED AT 19:13:40 ON 20 NOV 2003)

FILE 'REGISTRY' ENTERED AT 19:17:09 ON 20 NOV 2003

L1 STRUCTURE UPLOADED
L2 1 S L1
L3 19 S L1 FUL

FILE 'CAPLUS' ENTERED AT 19:18:29 ON 20 NOV 2003

L4 5 S L3
L5 STRUCTURE UPLOADED

FILE 'REGISTRY' ENTERED AT 19:32:10 ON 20 NOV 2003

L6 3021 S L5 FUL
L7 3003 S L6 NOT L4
L8 STRUCTURE UPLOADED
L9 0 S L8
L10 11 S L9 FUL